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* * * * * STN Columbus * * * * *

FILE 'HOME' ENTERED AT 08:42:24 ON 06 JUN 2007

=> file reg

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

0.21

0.21

FILE 'REGISTRY' ENTERED AT 08:42:34 ON 06 JUN 2007

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STRUCTURE FILE UPDATES: 5 JUN 2007 HIGHEST RN 936615-27-9

DICTIONARY FILE UPDATES: 5 JUN 2007 HIGHEST RN 936615-27-9

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH December 2, 2006

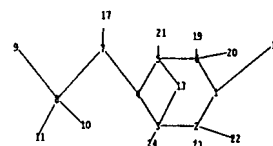
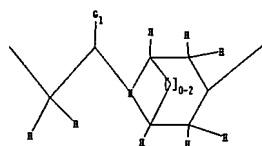
Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

<http://www.cas.org/support/stngen/stndoc/properties.html>

=>

Uploading C:\Program Files\Stnexp\Queries\10539106.str



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chain nodes :
7 8 9 10 11 12 17 19 20 21 22 23 24
ring nodes :
1 2 3 4 5 6 13
chain bonds :
1-12 2-22 2-23 3-24 4-7 5-21 6-19 6-20 7-8 7-17 8-9 8-10 8-11
ring bonds :
1-2 1-6 2-3 3-4 3-13 4-5 5-6 5-13
exact/norm bonds :
1-2 1-6 2-3 3-4 3-13 4-5 4-7 5-6 5-13 7-17
exact bonds :
1-12 2-22 2-23 3-24 5-21 6-19 6-20 7-8 8-9 8-10 8-11
isolated ring systems :
containing 1 :

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G1:C,H

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Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS
11:CLASS 12:CLASS 13:Atom 17:CLASS 19:CLASS 20:CLASS 21:CLASS 22:CLASS
23:CLASS 24:CLASS

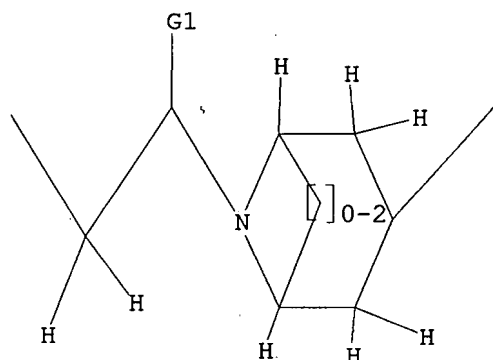
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L1 STRUCTURE UPLOADED

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L1 HAS NO ANSWERS

L1 STR



G1 C,H

Structure attributes must be viewed using STN Express query preparation.

=> s l1

SAMPLE SEARCH INITIATED 08:43:05 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 196 TO ITERATE

100.0% PROCESSED 196 ITERATIONS

4 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS: 3081 TO 4759

PROJECTED ANSWERS: 4 TO 200

L2 4 SEA SSS SAM L1

=> s l1 full

FULL SEARCH INITIATED 08:43:09 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 3815 TO ITERATE

100.0% PROCESSED 3815 ITERATIONS

133 ANSWERS

SEARCH TIME: 00.00.01

L3 133 SEA SSS FUL L1

=> file caplus

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

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172.31

FILE 'CAPLUS' ENTERED AT 08:43:13 ON 06 JUN 2007

USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.

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FILE COVERS 1907 - 6 Jun 2007 VOL 146 ISS 24
FILE LAST UPDATED: 5 Jun 2007 (20070605/ED)

Effective October 17, 2005, revised CAS Information Use Policies apply. They are available for your review at:

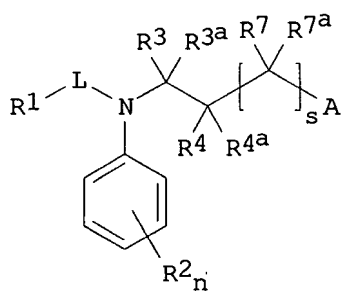
<http://www.cas.org/infopolicy.html>

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L4 28 L3

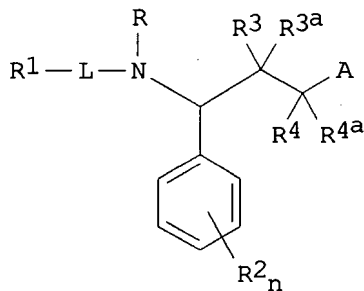
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L4 ANSWER 1 OF 28 CAPLUS COPYRIGHT 2007 ACS on STN
ACCESSION NUMBER: 2006:1285816 CAPLUS
DOCUMENT NUMBER: 146:45547
TITLE: Preparation of aryl bicyclo and spiro compounds as therapeutic modulators of CCR-5 activity
INVENTOR(S): Boman, Erik; Dahl, Russell; Delaet, Nancy G. J.; Ernst, Justin; Lum, Christopher; Sebo, Lubomir; Urban, Jan
PATENT ASSIGNEE(S): Kemia, Inc., USA
SOURCE: PCT Int. Appl., 235pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

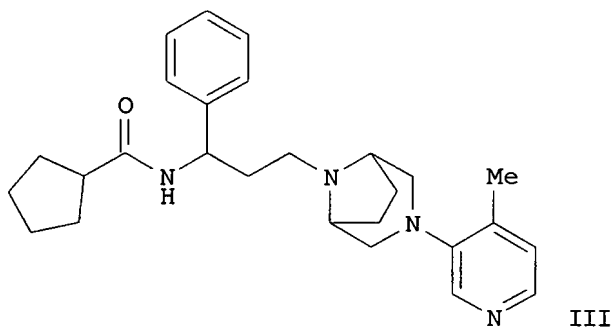
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WO 2006130426	A2	20061207	WO 2006-US20255	20060525
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RW:	AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM			
PRIORITY APPLN. INFO.:			US 2005-685147P	P 20050527
			US 2006-785090P	P 20060322
OTHER SOURCE(S):	MARPAT 146:45547			
GI				



I



II



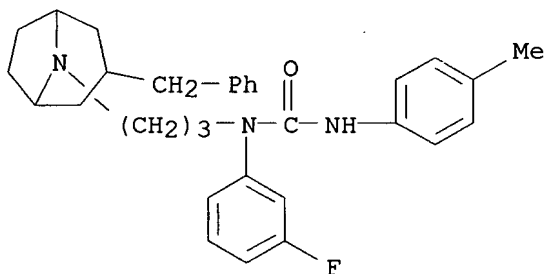
III

AB The present invention relates to low mol. weight compds., including compds. of Formulas I and II, and pharmaceutical compns. thereof, useful as modulators of CCR-5 activity (no biol. activity given). For I and II, A = a substituted spiro, bicyclo, or piperazinyl ring; R1 = (un)substituted alkyl, alkenyl, alkynyl, aryl, aralkyl, heterocyclyl or heterocyclylalkyl group; R2= halo or (un)substituted C1-C4 alkyl; R3, R3a, R4, R4a, R7, and R7a = H, halo, or (un)substituted C1-6 alkyl or C1-4 alkoxy group; and n = 0-5. The invention further relates to the use of such compds. and compns. in treating disorders mediated by CCR-5 such as viral infections and inflammatory diseases. Preparation methods for I and II are disclosed. For example, III is prepared by reacting 8-boc-3,8-diaza-3-(4-methylpyrid-3-yl)bicyclo[3.2.1]octane (preparation given) and (S)-tert-Bu 3-oxo-1-phenylpropylcarbamate to give an amine intermediate which is subsequently reacted with cyclopentyl carbonyl chloride.

IT 916454-94-9P 916454-95-0P 916454-96-1P
916454-97-2P 916458-71-4P, 1-Acetyl-N-[3-(3-benzyl-8-azabicyclo[3.2.1]octan-8-yl)propyl]-N-phenylpiperidine-4-carboxamide
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(drug candidate; preparation of aryl bicyclo and spiro compds. as therapeutic modulators of CCR-5 activity)

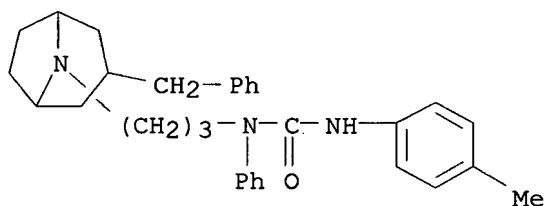
RN 916454-94-9 CAPLUS

CN Urea, N-(3-fluorophenyl)-N'-(4-methylphenyl)-N-[3-[3-(phenylmethyl)-8-azabicyclo[3.2.1]oct-8-yl]propyl]- (CA INDEX NAME)



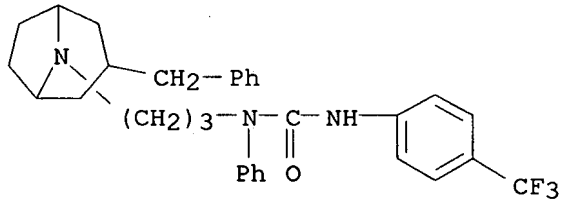
RN 916454-95-0 CAPLUS

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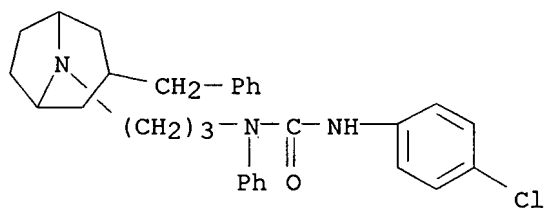
RN 916454-96-1 CAPLUS

CN Urea, N-phenyl-N-[3-[3-(phenylmethyl)-8-azabicyclo[3.2.1]oct-8-yl]propyl]-N'-(4-(trifluoromethyl)phenyl)- (CA INDEX NAME)



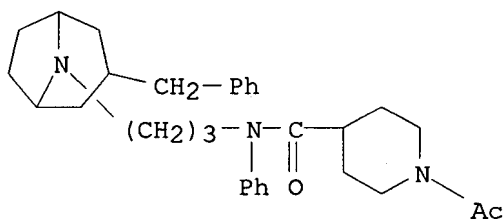
RN 916454-97-2 CAPLUS

CN Urea, N'-(4-chlorophenyl)-N-phenyl-N-[3-[3-(phenylmethyl)-8-azabicyclo[3.2.1]oct-8-yl]propyl]- (CA INDEX NAME)



RN 916458-71-4 CAPLUS

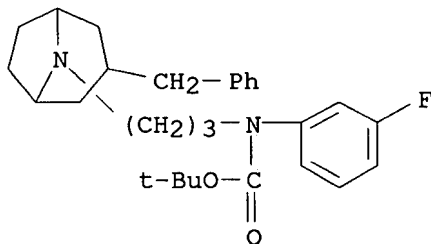
CN 4-Piperidinecarboxamide, 1-acetyl-N-phenyl-N-[3-[3-(phenylmethyl)-8-azabicyclo[3.2.1]oct-8-yl]propyl]- (CA INDEX NAME)



IT 916458-67-8P, tert-Butyl N-[3-(3-benzyl-8-azabicyclo[3.2.1]octan-8-yl)propyl](3-fluorophenyl)carbamate 916458-68-9P,
 N-[3-(3-Benzyl-8-azabicyclo[3.2.1]octan-8-yl)propyl]-3-fluoroaniline
 916458-69-0P, tert-Butyl N-[3-(3-benzyl-8-azabicyclo[3.2.1]octan-8-yl)propyl](phenyl)carbamate 916458-70-3P, N-[3-(3-Benzyl-8-azabicyclo[3.2.1]octan-8-yl)propyl]aniline
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation of aryl bicyclo and spiro compds. as therapeutic modulators of CCR-5 activity)

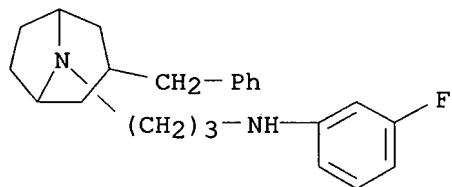
RN 916458-67-8 CAPLUS

CN Carbamic acid, N-(3-fluorophenyl)-N-[3-[3-(phenylmethyl)-8-azabicyclo[3.2.1]oct-8-yl]propyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)



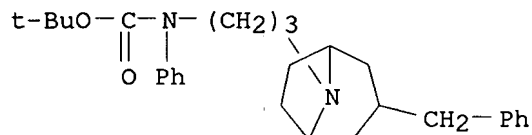
RN 916458-68-9 CAPLUS

CN 8-Azabicyclo[3.2.1]octane-8-propanamine, N-(3-fluorophenyl)-3-(phenylmethyl)- (CA INDEX NAME)

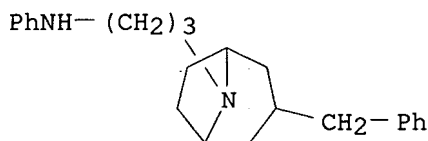


RN 916458-69-0 CAPLUS

CN Carbamic acid, N-phenyl-N-[3-[3-(phenylmethyl)-8-azabicyclo[3.2.1]oct-8-yl]propyl]-, 1,1-dimethylethyl ester (CA INDEX NAME)



RN 916458-70-3 CAPLUS
CN 8-Azabicyclo[3.2.1]octane-8-propanamine, N-phenyl-3-(phenylmethyl)- (CA
INDEX NAME)



L4 ANSWER 2 OF 28 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2006:1108680 CAPLUS

DOCUMENT NUMBER: 146:19364

TITLE: Synthesis of dopamine transporter selective
3-diarylmethoxymethyl-8-arylalkyl-8-
azabicyclo[3.2.1]octane derivatives

AUTHOR(S): Zhang, Suhong; Izenwasser, Sari; Wade, Dean; Xu,
Liang; Trudell, Mark L.

CORPORATE SOURCE: Department of Chemistry, University of New Orleans,
USA

SOURCE: Bioorganic & Medicinal Chemistry (2006), 14(23),
7943-7952

CODEN: BMECEP; ISSN: 0968-0896

PUBLISHER: Elsevier Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 146:19364

AB A series of diarylmethoxymethyltropane-GBR hybrid analogs with all three possible stereochem. orientations at C3 were synthesized and evaluated at dopamine and serotonin transporters. The 3 α derivs. were found to be the most potent compds. with the 3 α -di(4-fluorophenyl)methoxymethyl-8-(3-phenylpropyl)-8-azabicyclo[3.2.1]octane 15b (K_i = 5 nM) being the most potent compound of the series. The corresponding 3-di(4-fluorophenyl)-methoxymethyl-8-(3-phenylpropyl)-8-azabicyclo[3.2.1]oct-2-ene 12b (K_i = 12 nM) was slightly less potent than the 3 α -analog, while the 3 β -di(4-fluorophenyl)methoxymethyl-8-(3-phenylpropyl)-8-azabicyclo[3.2.1]octane 23b (K_i = 78 nM) exhibited only modest affinity for the dopamine transporter. Only the 3 α -analog 15b (SERT/DAT = 48) exhibited higher SERT/DAT selectivity than GBR 12909. These results indicate that the dopamine transporter can tolerate some variability in proximity of the benzhydryl ether to the basic nitrogen atom of the tropane without loss in potency. In addition, the structure-activity data for these tropane-GBR 12909 hybrid analogs support previous findings that the stereochem. and conformational effects imparted by unsatn. at C3 are important for dopamine transporter selectivity over the serotonin transporter.

IT 915098-04-3P 915098-06-5P 915217-69-5P
915217-71-9P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
(Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
(Uses)

(dopamine transporter selective azabicyclooctane derivs.)

RN 915098-04-3 CAPLUS

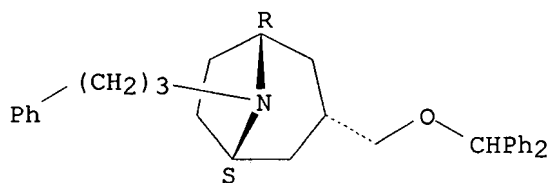
CN 8-Azabicyclo[3.2.1]octane, 3-[(diphenylmethoxy)methyl]-8-(3-phenylpropyl)-
, (3-endo)-, ethanedioate (1:1) (CA INDEX NAME)

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CRN 915098-03-2

CMF C30 H35 N O

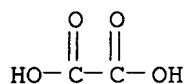
Relative stereochemistry.



CM 2

CRN 144-62-7

CMF C2 H2 O4



RN 915098-06-5 CAPLUS

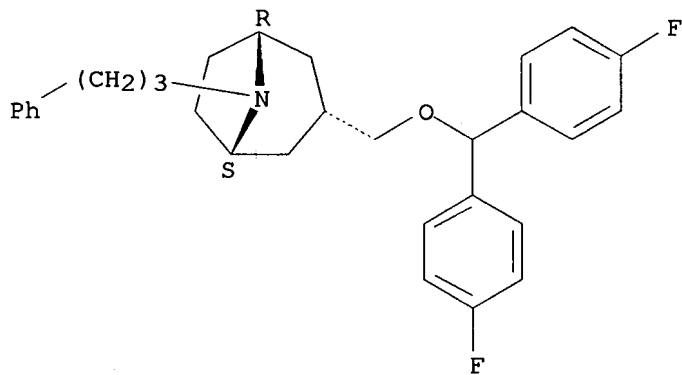
CN 8-Azabicyclo[3.2.1]octane, 3-[[bis(4-fluorophenyl)methoxy]methyl]-8-(3-phenylpropyl)-, (3-endo)-, ethanedioate (1:1) (CA INDEX NAME)

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CRN 915098-05-4

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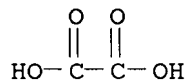
Relative stereochemistry.



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CRN 144-62-7

CMF C2 H2 O4



RN 915217-69-5 CAPLUS

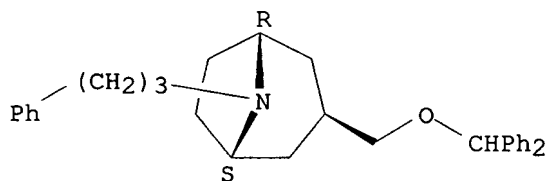
CN 8-Azabicyclo[3.2.1]octane, 3-[(diphenylmethoxy)methyl]-8-(3-phenylpropyl)-, ethanedioate (1:1), (3-exo)- (CA INDEX NAME)

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CRN 915217-68-4

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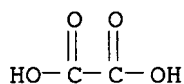
Relative stereochemistry.



CM 2

CRN 144-62-7

CMF C2 H2 O4



RN 915217-71-9 CAPLUS

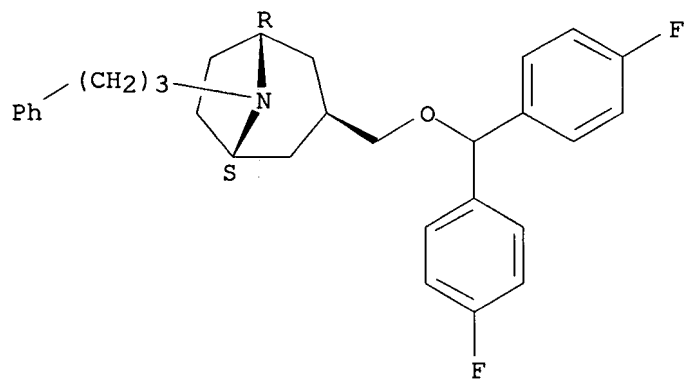
CN 8-Azabicyclo[3.2.1]octane, 3-[[bis(4-fluorophenyl)methoxy)methyl]-8-(3-phenylpropyl)-, ethanedioate (1:1), (3-exo)- (CA INDEX NAME)

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CRN 915217-70-8

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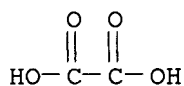
Relative stereochemistry.



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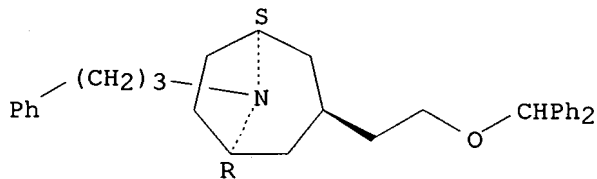
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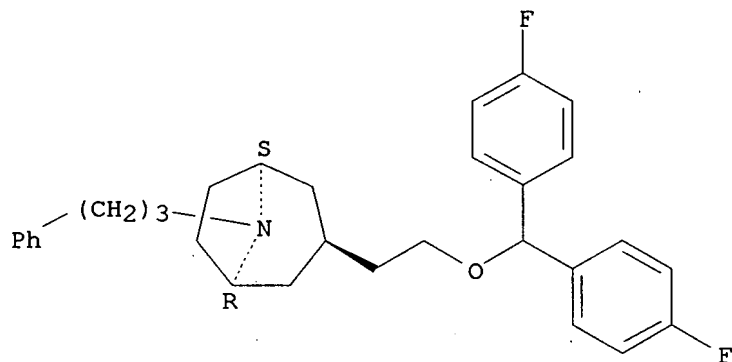
IT 548459-03-6 548459-05-8
 RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
 (Biological study); USES (Uses)
 (dopamine transporter selective azabicyclooctane derivs.)
 RN 548459-03-6 CAPLUS
 CN 8-Azabicyclo[3.2.1]octane, 3-[2-(diphenylmethoxy)ethyl]-8-(3-phenylpropyl)-
 , (3-endo)- (CA INDEX NAME)

Relative stereochemistry.



RN 548459-05-8 CAPLUS
 CN 8-Azabicyclo[3.2.1]octane, 3-[2-[bis(4-fluorophenyl)methoxy]ethyl]-8-(3-phenylpropyl)-, (3-endo)- (CA INDEX NAME)

Relative stereochemistry.



REFERENCE COUNT: 31 THERE ARE 31 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 3 OF 28 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2005:451115 CAPLUS

DOCUMENT NUMBER: 143:7605

TITLE: A preparation of azabicyclo[3.2.1]octane derivatives, useful as M3 muscarinic acetylcholine receptor antagonists

INVENTOR(S): Wan, Zehong; Yan, Hongxing; Palovich, Michael R.; Laine, Dramane I.; Lee, Dennis; Stavenger, Robert A.; Goodman, Krista B.; Hilfiker, Mark A.; Cui, Haifeng; Viet, Andrew W.; Marino, Joseph P.

PATENT ASSIGNEE(S): Glaxo Group Limited, UK

SOURCE: PCT Int. Appl., 48 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005046586	A2	20050526	WO 2004-US36663	20041104
WO 2005046586	A3	20050728		
WO 2005046586	A8	20050901		
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RW:	BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
EP 1682142	A2	20060726	EP 2004-810294	20041104
R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK, HR, IS			
JP 2007510731	T	20070426	JP 2006-539633	20041104
PRIORITY APPLN. INFO.:			US 2003-517243P	P 20031104
			WO 2004-US36663	W 20041104
OTHER SOURCE(S):	CASREACT 143:7605; MARPAT 143:7605			
GI				

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The invention relates to a preparation of azabicyclo[3.2.1]octane derivs. of formula I•X- [wherein: X- is an anion; R1 is alkyl, alkenyl, alkylcycloalkyl, or alkyl-OMe, etc.; R2 is (cyclo)alkyl, heterocycloalkyl, or cycloalkylalkyl, etc.], useful as M3 muscarinic acetylcholine receptor antagonists (no biol. data). For instance, quaternary azabicyclo[3.2.1]octane derivative II•Br- was prepared via quaternization of N-methylazabicyclo[3.2.1]octane derivative III by cyclopropylmethyl bromide with a yield of 51%.

IT 852436-02-3P 852460-99-2P 852461-00-8P
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852461-10-0P 852461-12-2P 852461-18-8P

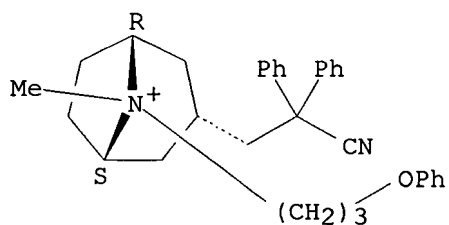
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of azabicyclo[3.2.1]octane derivs. useful as M3 muscarinic acetylcholine receptor antagonists)

RN 852436-02-3 CAPLUS

CN 8-Azoniabicyclo[3.2.1]octane, 3-(2-cyano-2,2-diphenylethyl)-8-methyl-8-(3-phenoxypropyl)-, bromide, (3-endo,8-syn)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

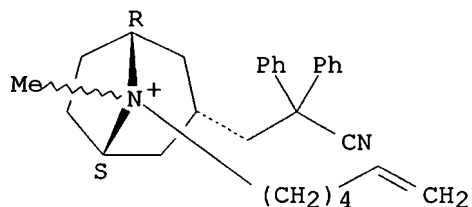


● Br⁻

RN 852460-99-2 CAPLUS

CN 8-Azoniabicyclo[3.2.1]octane, 3-(2-cyano-2,2-diphenylethyl)-8-(5-hexenyloxy)-8-methyl-, bromide, (3-endo,8-syn)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

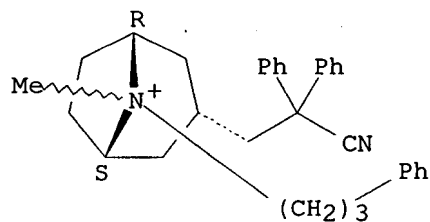


● Br⁻

RN 852461-00-8 CAPLUS

CN 8-Azoniabicyclo[3.2.1]octane, 3-(2-cyano-2,2-diphenylethyl)-8-methyl-8-(3-phenylpropyl)-, bromide, (3-endo,8-syn)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

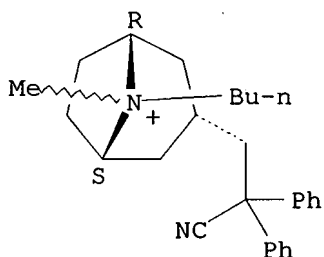


● Br⁻

RN 852461-03-1 CAPLUS

CN 8-Azoniabicyclo[3.2.1]octane, 8-butyl-3-(2-cyano-2,2-diphenylethyl)-8-methyl-, bromide, (3-endo,8-syn)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

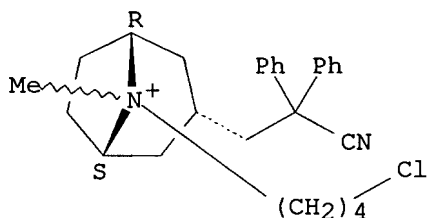


● Br⁻

RN 852461-04-2 CAPLUS

CN 8-Azoniabicyclo[3.2.1]octane, 8-(4-chlorobutyl)-3-(2-cyano-2,2-diphenylethyl)-8-methyl-, bromide, (3-endo,8-syn)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

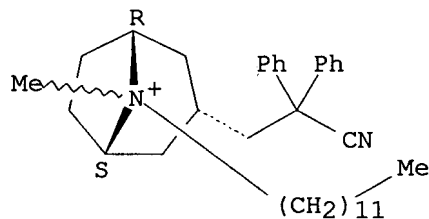


● Br⁻

RN 852461-05-3 CAPLUS

CN 8-Azoniabicyclo[3.2.1]octane, 3-(2-cyano-2,2-diphenylethyl)-8-dodecyl-8-methyl-, bromide, (3-endo,8-syn)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

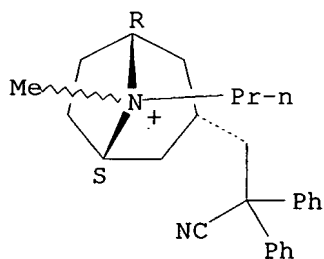


● Br⁻

RN 852461-10-0 CAPLUS

CN 8-Azoniabicyclo[3.2.1]octane, 3-(2-cyano-2,2-diphenylethyl)-8-methyl-8-propyl-, bromide, (3-endo,8-syn)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

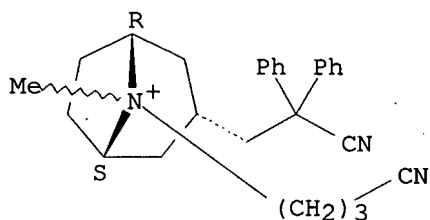


● Br⁻

RN 852461-12-2 CAPLUS

CN 8-Azoniabicyclo[3.2.1]octane, 3-(2-cyano-2,2-diphenylethyl)-8-(3-cyanopropyl)-8-methyl-, bromide, (3-endo,8-syn)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

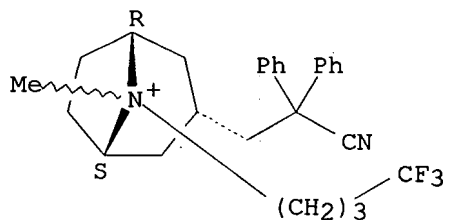


● Br⁻

RN 852461-18-8 CAPLUS

CN 8-Azoniabicyclo[3.2.1]octane, 3-(2-cyano-2,2-diphenylethyl)-8-methyl-8-(4,4,4-trifluorobutyl)-, bromide, (3-endo,8-syn)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



● Br⁻

IT 852435-97-3P 852435-99-5P 852436-00-1P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

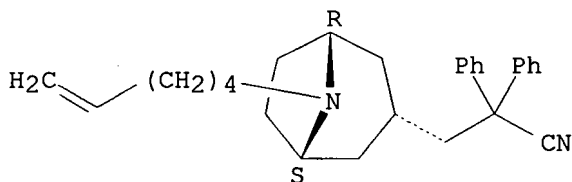
(preparation of azabicyclo[3.2.1]octane derivs. useful as M3 muscarinic acetylcholine receptor antagonists)

RN 852435-97-3 CAPLUS

CN 8-Azabicyclo[3.2.1]octane-3-propanenitrile, 8-(5-hexenyl)-α,α-

diphenyl-, (3-endo)- (9CI) (CA INDEX NAME)

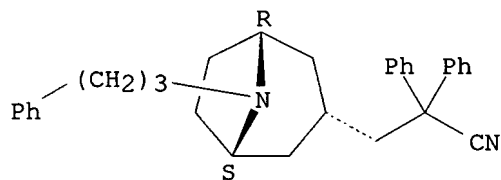
Relative stereochemistry.



RN 852435-99-5 CAPLUS

CN 8-Azabicyclo[3.2.1]octane-3-propanenitrile, α,α -diphenyl-8-(3-phenylpropyl)-, (3-endo)- (9CI) (CA INDEX NAME)

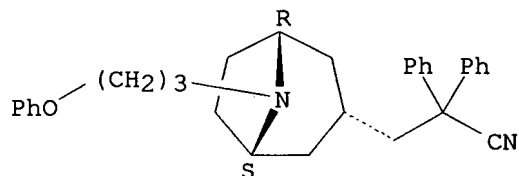
Relative stereochemistry.



RN 852436-00-1 CAPLUS

CN 8-Azabicyclo[3.2.1]octane-3-propanenitrile, 8-(3-phenoxypropyl)- α,α -diphenyl-, (3-endo)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



L4 ANSWER 4 OF 28 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2004:878395 CAPLUS

DOCUMENT NUMBER: 141:366230

TITLE: Preparation of heterocyclalkylbenzazolidinones as muscarinic M1 and M4 agonists.

INVENTOR(S): Kelly, Nicholas Michael; Koch, Kristian Norup; Tolf, Bo-Ragnar

PATENT ASSIGNEE(S): Acadia Pharmaceuticals Inc., USA

SOURCE: PCT Int. Appl., 92 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 3

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004089942	A2	20041021	WO 2004-US9859	20040330
WO 2004089942	A3	20041125		
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC,			

LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI,
 NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY,
 TJ, TM, TN, TR, TT, TZ, UA, UG, UZ, VC, VN, YU, ZA, ZM, ZW
 RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ,
 BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE,
 ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI,
 SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN,
 TD, TG

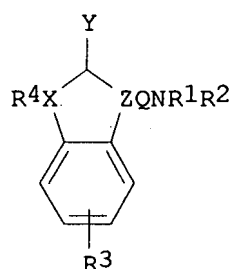
US 2003100545	A1	20030529	US 2002-262517	20020930
US 7087593	B2	20060808		
US 2004067931	A1	20040408	US 2003-408192	20030403
US 6951849	B2	20051004		

PRIORITY APPLN. INFO.:

US 2001-326754P	P	20011002
US 2002-262517	A	20020930
US 2003-406750	A2	20030402
US 2003-408192	A2	20030403

OTHER SOURCE(S): MARPAT 141:366230

GI



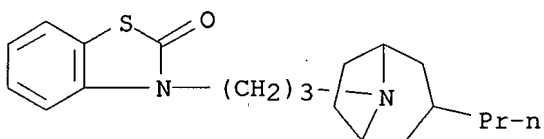
AB Title compds. [I; X = C, O, N, S; Z = CH, N; Y = O, N, S, tautomers thereof; Q = (CR6R7)nA, (CR6R7)p-CH=CH-(CR6R7)q, etc.; n, p, q = 0-5; A = null, C3-8 cycloalkyl; NR1R2 = (substituted) perhydroazocinyl, perhydroazepinyl, piperidinyl, pyrrolidinyl, azetidiny, aziridinyl, 8-azabicyclo[3.2.1]octyl; R3 = 0-4 of halo, OH, (substituted) alkyl, alkoxy, alkylidene, alkenyl, alkynyl, aryl, heteroaryl, cycloalkyl, heterocyclyl, alkylcarbonyl; R4 = H, (substituted) alkyl, cycloalkyl, alkenyl, alkynyl, aminomethyl, alkoxyethyl, alkylthiomethyl, etc.; R6, R7 = H, halo, OH, (substituted) alkyl, alkoxy, heteroalkyl, alkylidene, alkenyl, alkynyl, aryl, etc.], were prepared Thus, 3-(2-chloroethyl)-3H-benzothiazol-2-one (preparation given), 4-butylpiperidine, NaI, and K2CO3 were shaken in MeCN at 50° for 20 h to give 13% 3-[2-(4-butylpiperidin-1-yl)ethyl]-3H-benzothiazol-2-one. Tested I gave 63-115% efficacy at M1 receptors relative to carbachol.

IT 509147-52-8P 509147-53-9P 509147-54-0P
 509147-55-1P 676367-01-4P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
 (preparation of benzazolidinones as muscarinic M1 and M4 agonists)

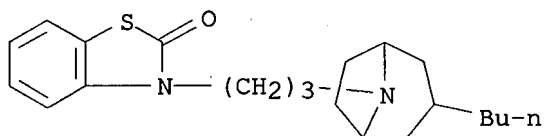
RN 509147-52-8 CAPLUS

CN 2(3H)-Benzothiazolone, 3-[3-(3-propyl-8-azabicyclo[3.2.1]oct-8-yl)propyl]-
 (9CI) (CA INDEX NAME)



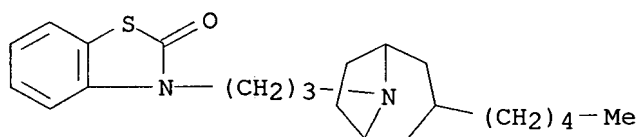
RN 509147-53-9 CAPLUS

CN 2(3H)-Benzothiazolone, 3-[3-(3-butyl-8-azabicyclo[3.2.1]oct-8-yl)propyl]-
(9CI) (CA INDEX NAME)



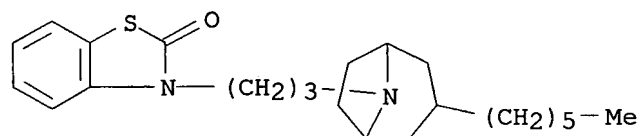
RN 509147-54-0 CAPLUS

CN 2(3H)-Benzothiazolone, 3-[3-(3-pentyl-8-azabicyclo[3.2.1]oct-8-yl)propyl]-
(9CI) (CA INDEX NAME)



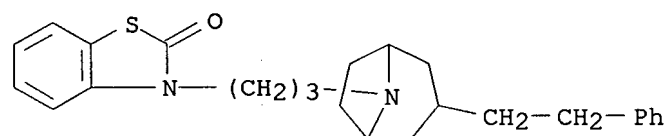
RN 509147-55-1 CAPLUS

CN 2(3H)-Benzothiazolone, 3-[3-(3-hexyl-8-azabicyclo[3.2.1]oct-8-yl)propyl]-
(9CI) (CA INDEX NAME)



RN 676367-01-4 CAPLUS

CN 2(3H)-Benzothiazolone, 3-[3-[3-(2-phenylethyl)-8-azabicyclo[3.2.1]oct-8-yl]propyl]- (9CI) (CA INDEX NAME)



L4 ANSWER 5 OF 28 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2004:293387 CAPLUS

DOCUMENT NUMBER: 140:303675

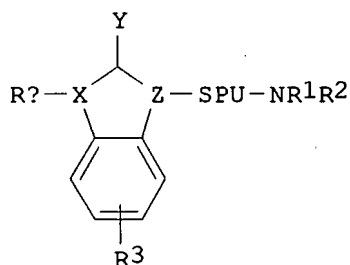
TITLE: Preparation of heterocyclalalkylbenzazolidinones as muscarinic M1 and M4 agonists.

INVENTOR(S): Kelly, Nicholas Michael; Koch, Kristian Norup; Tolf,

PATENT ASSIGNEE(S): Bo-Ragnar
 SOURCE: Acadia Pharmaceuticals, Inc., Den.
 U.S. Pat. Appl. Publ., 48 pp., Cont.-in-part of U.S.
 Ser. No. 262,517.
 CODEN: USXXCO
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 3
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2004067931	A1	20040408	US 2003-408192	20030403
US 6951849	B2	20051004		
US 2003100545	A1	20030529	US 2002-262517	20020930
US 7087593	B2	20060808		
WO 2004089942	A2	20041021	WO 2004-US9859	20040330
WO 2004089942	A3	20041125		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, UZ, VC, VN, YU, ZA, ZM, ZW RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
US 2006025402	A1	20060202	US 2005-188295	20050721
US 2006199799	A1	20060907	US 2006-418340	20060503
US 2006205785	A1	20060914	US 2006-418342	20060503
US 2006258707	A1	20061116	US 2006-490416	20060719
PRIORITY APPLN. INFO.: US 2001-326754P P 20011002 US 2002-262517 A2 20020930 US 2003-406750 A2 20030402 US 2003-408192 A2 20030403 US 2005-188295 A1 20050721				

OTHER SOURCE(S): MARPAT 140:303675
 GI



I

AB Title compds. [I; X = C, O, N, S; Z = CH, N; Y = O, N, S, tautomers thereof; SPU = spacer; N together with R1-2 form a heterocycle; R3 present 0-4 times = halo, OH, alkyl, etc.; Rx = absent, H, alkyl, etc.], are prepared Thus, 3-(2-chloroethyl)-3H-benzothiazol-2-one (preparation given), 4-butylpiperidine, NaI, and K2CO3 were shaken in MeCN at 50° for 20 h to give 13% 3-[2-(4-butylpiperidin-1-yl)ethyl]-3H-benzothiazol-2-one. Tested I gave 63-115% efficacy at M1 receptors relative to carbachol.

IT 509147-52-8P 509147-53-9P 509147-54-0P

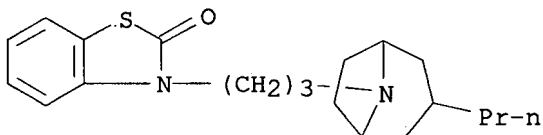
509147-55-1P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of benzazolidinones as muscarinic M1 and M4 agonists)

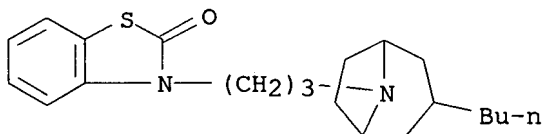
RN 509147-52-8 CAPLUS

CN 2(3H)-Benzothiazolone, 3-[3-(3-propyl-8-azabicyclo[3.2.1]oct-8-yl)propyl]-(9CI) (CA INDEX NAME)



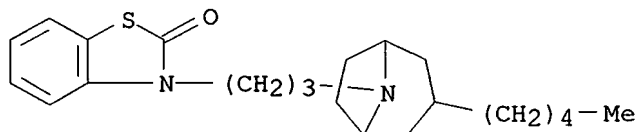
RN 509147-53-9 CAPLUS

CN 2(3H)-Benzothiazolone, 3-[3-(3-butyl-8-azabicyclo[3.2.1]oct-8-yl)propyl]-(9CI) (CA INDEX NAME)



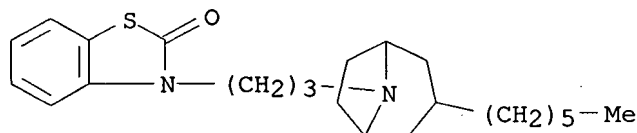
RN 509147-54-0 CAPLUS

CN 2(3H)-Benzothiazolone, 3-[3-(3-pentyl-8-azabicyclo[3.2.1]oct-8-yl)propyl]-(9CI) (CA INDEX NAME)



RN 509147-55-1 CAPLUS

CN 2(3H)-Benzothiazolone, 3-[3-(3-hexyl-8-azabicyclo[3.2.1]oct-8-yl)propyl]-(9CI) (CA INDEX NAME)



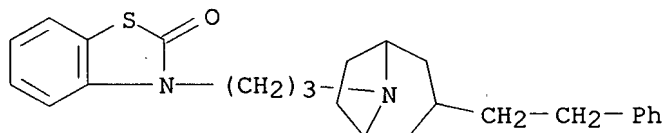
IT 676367-01-4P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of heterocyclalalkylbenzazolidinones as muscarinic M1 and M4 agonists)

RN 676367-01-4 CAPLUS

CN 2(3H)-Benzothiazolone, 3-[3-[3-(2-phenylethyl)-8-azabicyclo[3.2.1]oct-8-yl]propyl]-(9CI) (CA INDEX NAME)



REFERENCE COUNT: 33 THERE ARE 33 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 6 OF 28 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2004:214100 CAPLUS

DOCUMENT NUMBER: 141:396

TITLE: Discovery of N-propylurea 3-benzylpiperidines as selective CC chemokine receptor-3 (CCR3) antagonists

AUTHOR(S): Varnes, Jeffrey G.; Gardner, Daniel S.; Santella, Joseph B.; Duncia, John V.; Estrella, Melissa; Watson, Paul S.; Clark, Cheryl M.; Ko, Soo S.; Welch, Patricia; Covington, Maryanne; Stowell, Nicole; Wadman, Eric; Davies, Paul; Solomon, Kimberley; Newton, Robert C.; Trainor, George L.; Decicco, Carl P.; Wacker, Dean A.

CORPORATE SOURCE: Bristol-Myers Squibb Pharmaceutical Research Institute, Princeton, NJ, 08542-5400, USA

SOURCE: Bioorganic & Medicinal Chemistry Letters (2004), 14(7), 1645-1649
CODEN: BMCLE8; ISSN: 0960-894X

PUBLISHER: Elsevier Science B.V.

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 141:396

AB The discovery of novel and selective small mol. antagonists of the CC chemokine receptor-3 (CCR3) is presented. Simple conversion from a 4- to 3-benzylpiperidine gave improved selectivity for CCR3 over the serotonin 5HT2A receptor. Chiral resolution and exploration of mono- and disubstitution of the N-propylurea resulted in several 3-benzylpiperidine N-propylureas with CCR3 binding IC50s under 5 nM. Data from in vitro calcium mobilization and chemotaxis assays for these compds. ranged from high picomolar to low nanomolar EC50s and correlated well with antagonist binding IC50s.

IT 693256-78-9P 693788-77-1P

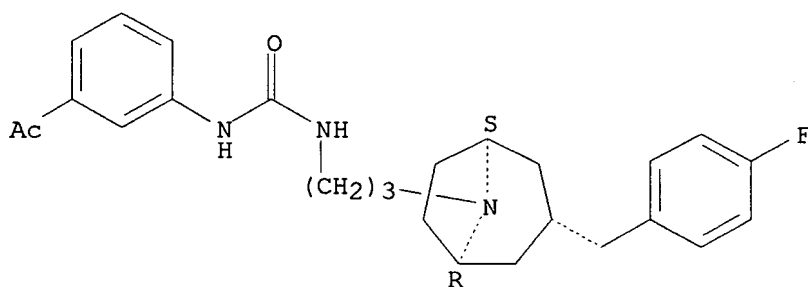
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(discovery of propylurea benzylpiperidines as selective CCR3 antagonists)

RN 693256-78-9 CAPLUS

CN Urea, N-(3-acetylphenyl)-N'-[3-[(3-exo)-3-[(4-fluorophenyl)methyl]-8-azabicyclo[3.2.1]oct-8-yl]propyl]- (9CI) (CA INDEX NAME)

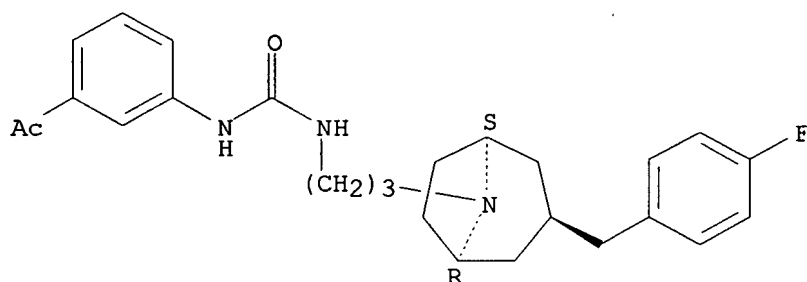
Relative stereochemistry.



RN 693788-77-1 CAPLUS

CN Urea, N-(3-acetylphenyl)-N'-[3-[(3-endo)-3-[(4-fluorophenyl)methyl]-8-azabicyclo[3.2.1]oct-8-yl]propyl]- (9CI) (CA INDEX NAME)

Relative stereochemistry.



REFERENCE COUNT: 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 7 OF 28 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2003:282333 CAPLUS

DOCUMENT NUMBER: 138:304284

TITLE: Preparation of heterocyclalkylbenzazolidinones as muscarinic M1 and M4 agonists.

INVENTOR(S): Kelly, Nicholas Michael; Koch, Kristian Norup; Tolf, Bo-ragnar

PATENT ASSIGNEE(S): Acadia Pharmaceuticals, Inc., USA

SOURCE: PCT Int. Appl., 90 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

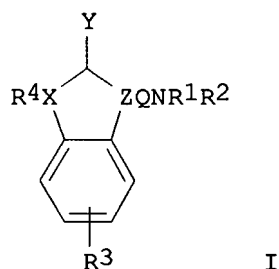
LANGUAGE: English

FAMILY ACC. NUM. COUNT: 3

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003028650	A2	20030410	WO 2002-US31308	20020930
WO 2003028650	A3	20030619		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				

AU 2002327810	A1	20030414	AU 2002-327810	20020930
EP 1432420	A2	20040630	EP 2002-763824	20020930
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK				
CN 1561212	A	20050105	CN 2002-819444	20020930
JP 2005510473	T	20050421	JP 2003-531986	20020930
BR 2002013611	A	20051220	BR 2002-13611	20020930
RU 2288919	C2	20061210	RU 2004-113451	20020930
NZ 531550	A	20061222	NZ 2002-531550	20020930
NO 2004001317	A	20040629	NO 2004-1317	20040330
ZA 2004002609	A	20050509	ZA 2004-2609	20040401
PRIORITY APPLN. INFO.:			US 2001-326754P	P 20011002
OTHER SOURCE(S):			WO 2002-US31308	W 20020930
GI			MARPAT 138:304284	

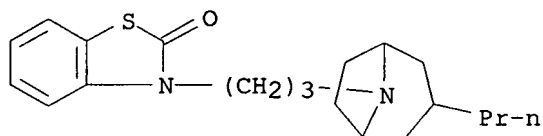


AB Title compds. [I; X = C, O, N, S; Z = CH, N; Y = O, N, S, tautomers thereof; Q = (CR6R7)nA, C3-8 cycloalkyl; n = 1-5; A = null, C3-8 cycloalkyl; NR1R2 = (substituted) perhydroazocinyl, perhydroazepinyl, piperidinyl, pyrrolidinyl, azetidiny, aziridinyl, 8-azabicyclo[3.2.1]octyl; R3 = 0-4 of halo, OH, (substituted) alkyl, alkoxy, alkylidene, alkenyl, alkynyl, aryl, heteroaryl, cycloalkyl, heterocyclyl, alkylcarbonyl; R4 = H, (substituted) alkyl, cycloalkyl, alkenyl, alkynyl, aminomethyl, alkoxyethyl, alkylthiomethyl, etc.], were prepared Thus, 3-(2-chloroethyl)-3H-benzothiazol-2-one (preparation given), 4-butylpiperidine, NaI, and K2CO3 were shaken in MeCN at 50° for 20 h to give 13% 3-[2-(4-butylpiperidin-1-yl)ethyl]-3H-benzothiazol-2-one. Tested I gave 63-115% efficacy at M1 receptors relative to carbachol.

IT 509147-52-8P 509147-53-9P 509147-54-0P
509147-55-1P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of benzazolidinones as muscarinic M1 and M4 agonists)

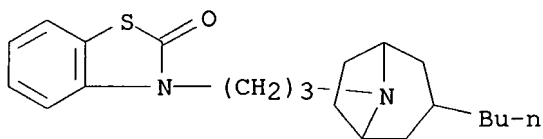
RN 509147-52-8 CAPLUS

CN 2(3H)-Benzothiazolone, 3-[3-(3-propyl-8-azabicyclo[3.2.1]oct-8-yl)propyl]-(9CI) (CA INDEX NAME)



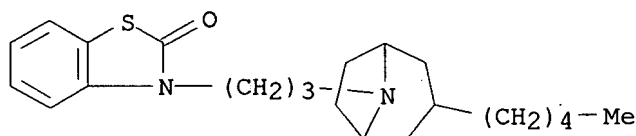
RN 509147-53-9 CAPLUS

CN 2(3H)-Benzothiazolone, 3-[3-(3-butyl-8-azabicyclo[3.2.1]oct-8-yl)propyl]-(9CI) (CA INDEX NAME)



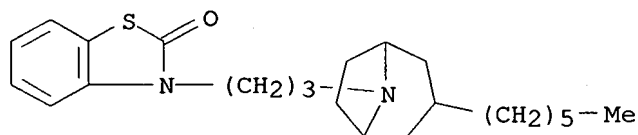
RN 509147-54-0 CAPLUS

CN 2(3H)-Benzothiazolone, 3-[3-(3-pentyl-8-azabicyclo[3.2.1]oct-8-yl)propyl]-
(9CI) (CA INDEX NAME)



RN 509147-55-1 CAPLUS

CN 2(3H)-Benzothiazolone, 3-[3-(3-hexyl-8-azabicyclo[3.2.1]oct-8-yl)propyl]-
(9CI) (CA INDEX NAME)



L4 ANSWER 8 OF 28 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2003:189370 CAPLUS

DOCUMENT NUMBER: 139:52839

TITLE: Synthesis of dopamine transporter selective
3-{2-(Diarylmethoxyethylidene))-8-alkylaryl-8-
azabicyclo[3.2.1]octanes

AUTHOR(S): Bradley, Amy L.; Izenwasser, Sari; Wade, Dean;
Cararas, Shaine; Trudell, Mark L.

CORPORATE SOURCE: Department of Chemistry, University of New Orleans,
New Orleans, LA, 70148, USA

SOURCE: Bioorganic & Medicinal Chemistry Letters (2003),
13(4), 629-632

CODEN: BMCLE8; ISSN: 0960-894X

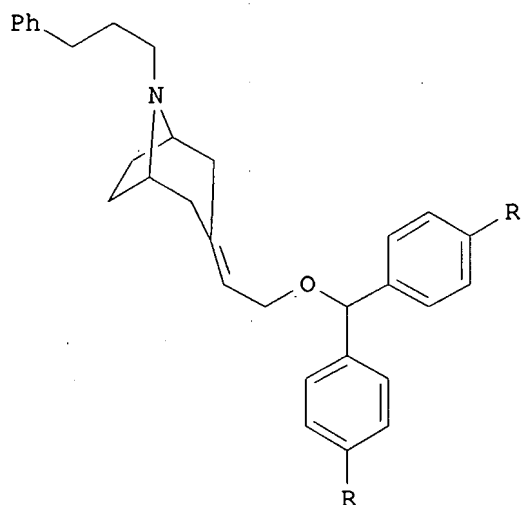
PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 139:52839

GI



I

AB A series of 3-{2-(diarylmethoxyethylidene)}-8-alkylaryl-8-azabicyclo[3.2.1]octanes was synthesized and the binding affinities of the compds. were determined at the dopamine and serotonin transporters. The 8-phenylpropyl analogs I [R = H (K_i =4.1 nM); R = F (K_i =3.7 nM)] were the most potent compds. of the series with binding affinities 3 times greater than GBR-12909. In addition, I (R = H; SERT/DAT=327) was over 300-fold more selective for the dopamine transporter than the serotonin transporter.

IT 548459-04-7P 548459-06-9P 548459-08-1P
548459-10-5P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(stereoselective preparation, dopamine and serotonin transporter affinities, and SAR of (diarylmethoxyethyl)azabicyclooctanes via reduction of azabicyclooctaneacetate followed by alkylation with benzhydryl chlorides)

RN 548459-04-7 CAPLUS

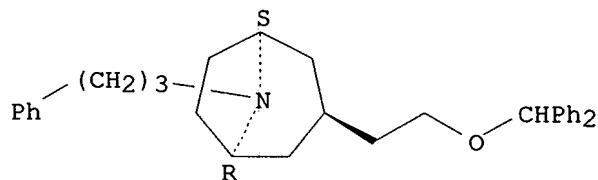
CN 8-Azabicyclo[3.2.1]octane, 3-[2-(diphenylmethoxy)ethyl]-8-(3-phenylpropyl)-, (3-endo)-, ethanedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 548459-03-6

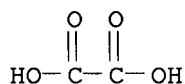
CMF C31 H37 N O

Relative stereochemistry.



CM 2

CRN 144-62-7
CMF C2 H2 O4



RN 548459-06-9 CAPLUS

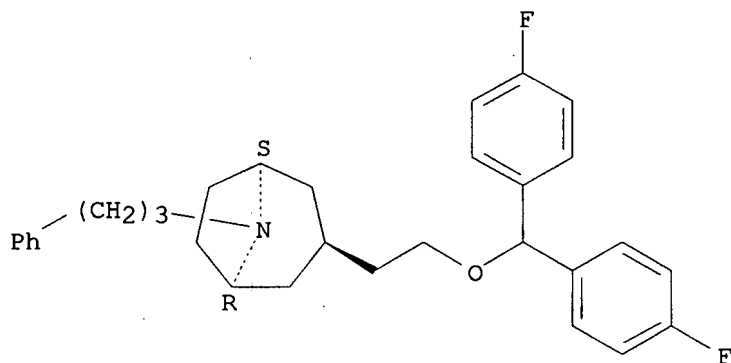
CN 8-Azabicyclo[3.2.1]octane, 3-[2-[bis(4-fluorophenyl)methoxy]ethyl]-8-(3-phenylpropyl)-, (3-endo)-, ethanedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 548459-05-8

CMF C31 H35 F2 N O

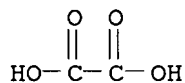
Relative stereochemistry.



CM 2

CRN 144-62-7

CMF C2 H2 O4



RN 548459-08-1 CAPLUS

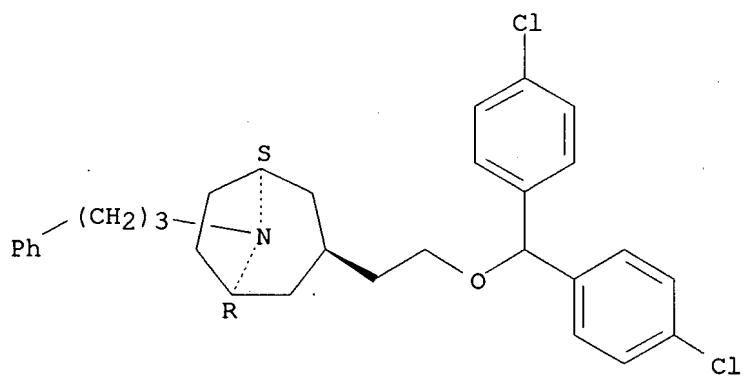
CN 8-Azabicyclo[3.2.1]octane, 3-[2-[bis(4-chlorophenyl)methoxy]ethyl]-8-(3-phenylpropyl)-, (3-endo)-, ethanedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 548459-07-0

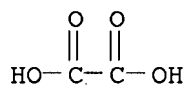
CMF C31 H35 Cl2 N O

Relative stereochemistry.



CM 2

CRN 144-62-7
CMF C2 H2 O4



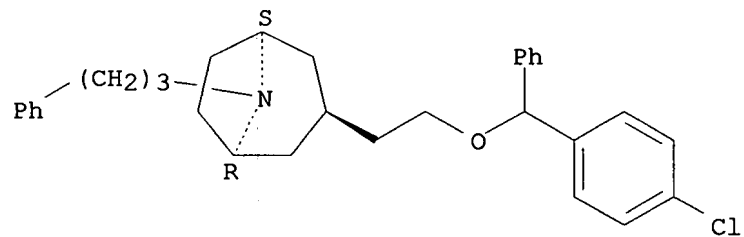
RN 548459-10-5 CAPLUS

CN 8-Azabicyclo[3.2.1]octane, 3-[2-[(4-chlorophenyl)phenylmethoxy]ethyl]-8-(3-phenylpropyl)-, (3-endo)-, ethanedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

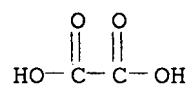
CRN 548459-09-2
CMF C31 H36 Cl N O

Relative stereochemistry.



CM 2

CRN 144-62-7
CMF C2 H2 O4



REFERENCE COUNT:

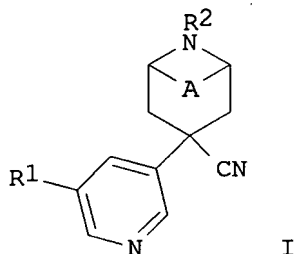
24

THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 9 OF 28 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2003:98104 CAPLUS
DOCUMENT NUMBER: 138:137175
TITLE: Preparation of 3-cyano-3-pyridylazabicyclo[3.2.1]octanes as insecticides, acaricides, and nematocides.
INVENTOR(S): Salmon, Roger
PATENT ASSIGNEE(S): Syngenta Limited, UK
SOURCE: Brit. UK Pat. Appl., 25 pp.
CODEN: BAXXDU
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
GB 2378181	A	20030205	GB 2002-15429	20020703
PRIORITY APPLN. INFO.:			GB 2001-17032	A 20010712
OTHER SOURCE(S):	MARPAT	138:137175		
GI				



AB Title compds. I;. Thus, 8-benzyl-exo-3-cyano-8-azabicyclo[3.2.1]octane and 3,5-dibromopyridine in THF were treated with Li(SiMe₃)₂ to give 8-benzyl-exo-3-(5-bromopyrid-3-yl)-endo-3-cyano-8-azabicyclo[3.2.1]octane. The latter with MeI in Et₂O/THF at -30° was treated with MeLi followed by warming to room temperature to give 8-benzyl-endo-3-cyano-exo-3-(5-methylpyrid-3-yl)-8-azabicyclo[3.2.1]octane. Several I at 500 ppm gave 80-100% control of Myzus persicae on cabbage leaves.

IT 494767-63-4P

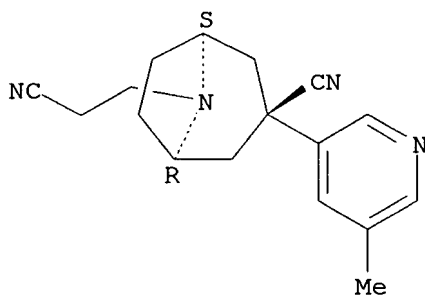
RL: AGR (Agricultural use); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of cyanopyridylazabicyclooctanes as insecticides, acaricides, and nematocides)

RN 494767-63-4 CAPLUS

CN 8-Azabicyclo[3.2.1]octane-8-propanenitrile, 3-cyano-3-(5-methyl-3-pyridinyl)-, (3-endo)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 10 OF 28 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2003:59634 CAPLUS

DOCUMENT NUMBER: 138:73416

TITLE: Preparation of pyridinyl-8-azabicyclics for use as pesticides

INVENTOR(S): Salmon, Roger; Bacon, David Philip

PATENT ASSIGNEE(S): Syngenta Limited, UK

SOURCE: Brit. UK Pat. Appl., 27 pp.

CODEN: BAXXDU

DOCUMENT TYPE: Patent

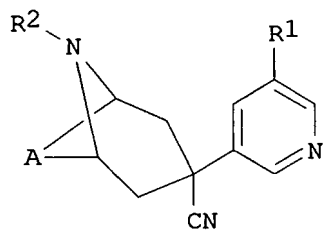
LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

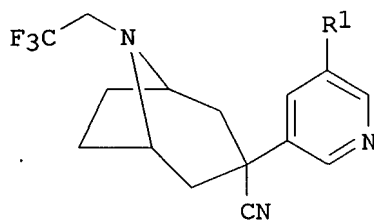
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
GB 2372744	A	20020904	GB 2002-823	20020115
PRIORITY APPLN. INFO.:			GB 2001-1226	A 20010117
OTHER SOURCE(S):	MARPAT	138:73416		

GI



I



II

AB Pyridinyl substituted azabicyclic compds., such as I [A = CH₂CH₂, CH:CH; R₁ = C₂-10-alkynyl; R₂ = H, CHO, carboxyl, alkyl, alkoxy, alkenyloxy, aryl, heteroaryl, etc.]. Thus, endo-3-cyano-8-(2,2,2-trifluoroethyl)-exo-3-[5-(trimethylsilylethynyl)pyrid-3-yl]-8-azabicyclo[3.2.1]octane II (R₁ = C.tplbond.CSiMe₃) was prepared by reaction of HC.tplbond.CSiMe₃ with the corresponding bromide II (R₁ = Br) using (Ph₃P)₂PdCl₂, CuI and Et₃N in a sealed glass carius tube and heated to 60° for 18 h. The prepared azabicyclics were assayed for their insecticidal activity against peach aphid, i.e. Myzus persicae, by determining mortality rate of a 500 ppm by weight

composition of each of the azabicyclics in an acetone/ethanol/water solution

IT 481696-05-3P 481696-14-4P 481696-15-5P

RL: AGR (Agricultural use); BSU (Biological study, unclassified); SPN

(Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES

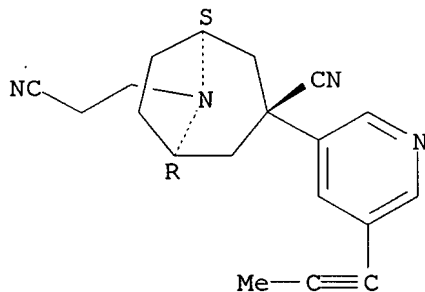
(Uses)

(preparation of pyridinyl-8-azabicyclo[3.2.1]octanes for use as pesticides)

RN 481696-05-3 CAPLUS

CN 8-Azabicyclo[3.2.1]octane-8-propanenitrile, 3-cyano-3-[5-(1-propynyl)-3-pyridinyl]-, (3-endo)- (9CI) (CA INDEX NAME)

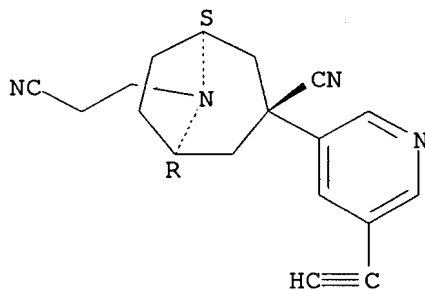
Relative stereochemistry.



RN 481696-14-4 CAPLUS

CN 8-Azabicyclo[3.2.1]octane-8-propanenitrile, 3-cyano-3-(5-ethynyl-3-pyridinyl)-, (3-endo)- (9CI) (CA INDEX NAME)

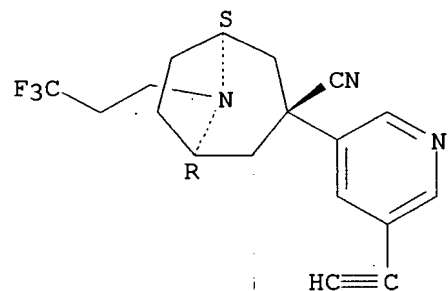
Relative stereochemistry.



RN 481696-15-5 CAPLUS

CN 8-Azabicyclo[3.2.1]octane-3-carbonitrile, 3-(5-ethynyl-3-pyridinyl)-8-(3,3,3-trifluoropropyl)-, (3-endo)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



L4 ANSWER 11 OF 28 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2002:555491 CAPLUS

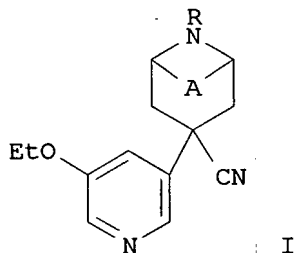
DOCUMENT NUMBER: 137:109215

TITLE: Preparation of 8-azabicyclo[3.2.1]octanes as insecticides

INVENTOR(S): Salmon, Roger

PATENT ASSIGNEE(S): Syngenta Limited, UK
 SOURCE: PCT Int. Appl., 26 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002057263	A1	20020725	WO 2002-GB154	20020115
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2002219384	A1	20020730	AU 2002-219384	20020115
PRIORITY APPLN. INFO.:			GB 2001-1229	A 20010117
			GB 2001-17033	A 20010712
			WO 2002-GB154	W 20020115
OTHER SOURCE(S):		MARPAT 137:109215		
GI				



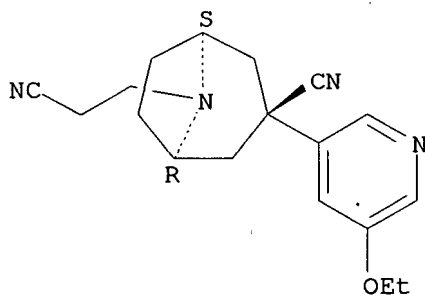
AB The title compds. I (A = CH₂-CH₂- or -CH=CH-; R = H, CHO, COOC₁-C₁₀ alkyl, optionally substituted C₂-C₁₀ alkyl, substituted Me, optionally substituted C₁-C₁₀ alkoxy, optionally substituted C₂-C₁₀ alkenyloxy, optionally substituted aryl, optionally substituted heteroaryl, optionally substituted C₂-C₁₀ alkenyl, optionally substituted C₃-C₁₀ alkynyl or optionally substituted C₃-C₇ cycloalkyl) and their acid addition salts, quaternary ammonium salts, salts and N-oxides were prepared as insecticides. Thus, 8-benzyl-exo-3-(5-chloro-3-pyridyl)-endo-3-cyano-8-azabicyclo[3.2.1]octane was treated with EtONa to give 8-benzyl-exo-3-(5-ethoxy-3-pyridyl)-endo-3-cyano-8-azabicyclo[3.2.1]octane (II). II had 80-100% mortality against *Myzus persicae* at 500 ppm.

IT 443640-57-1P
 RL: BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
 (preparation of 8-azabicyclo[3.2.1]octanes as insecticides)

RN 443640-57-1 CAPLUS

CN 8-Azabicyclo[3.2.1]octane-8-propanenitrile, 3-cyano-3-(5-ethoxy-3-pyridinyl)-, (3-endo)- (9CI) (CA INDEX NAME)

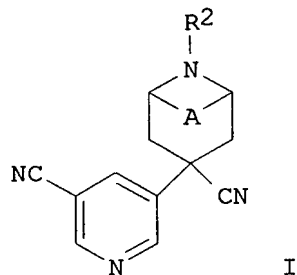
Relative stereochemistry.



REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 12 OF 28 CAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 2002:555490 CAPLUS
 DOCUMENT NUMBER: 137:125100
 TITLE: Bicyclic amines as insecticides
 INVENTOR(S): Salmon, Roger
 PATENT ASSIGNEE(S): Syngenta Limited, UK
 SOURCE: PCT Int. Appl., 30 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002057262	A2	20020725	WO 2002-GB152	20020115
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GH, GM, HR, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2002219383	A1	20020730	AU 2002-219383	20020115
PRIORITY APPLN. INFO.:			GB 2001-1228	A 20010117
			GB 2001-17035	A 20010712
			WO 2002-GB152	W 20020115
OTHER SOURCE(S):			MARPAT 137:125100	
GI				



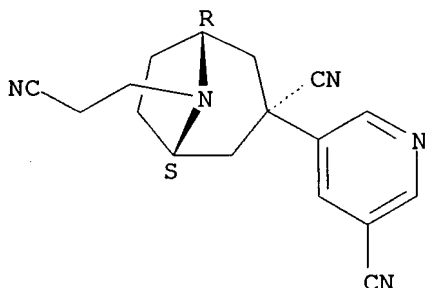
AB A compound of formula (I) wherein A is -CH₂-CH₂- or -CH=CH-; R₂ is hydrogen, CHO, COOC₁-C₁₀ alkyl, optionally substituted C₂-C₁₀ alkyl, substituted Me, optionally substituted C₁-C₁₀ alkoxy, optionally substituted C₂-C₁₀ alkenyloxy, optionally substituted aryl, optionally substituted heteroaryl, optionally substituted C₂-C₁₀ alkenyl, optionally substituted C₃-C₁₀ alkynyl or optionally substituted C₃-C₇ cycloalkyl; and acid addition salts, quaternary ammonium salts and N-oxides derived therefrom. The compds. are useful as insecticides.

IT 443925-07-3P
 RL: AGR (Agricultural use); IMF (Industrial manufacture); BIOL (Biological study); PREP (Preparation); USES (Uses)
 (insecticide; preparation of bicyclic amines as insecticides)

RN 443925-07-3 CAPLUS

CN 8-Azabicyclo[3.2.1]octane-8-propanenitrile, 3-cyano-3-(5-cyano-3-pyridinyl)-, (3-endo)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



L4 ANSWER 13 OF 28 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2002:256232 CAPLUS

DOCUMENT NUMBER: 136:294857

TITLE: Preparation of nitrogen-containing compounds as the active ingredient of CCR3 inhibitors

INVENTOR(S): Takahashi, Toshiya; Imaoka, Takayuki; Tomioka, Hiroki; Hatakeyama, Daigo; Nitta, Aiko; Kaneko, Masayuki; Takizawa, Satoko; Torii, Yuichi; Morihira, Koichiro; Morokata, Tatsuaki

PATENT ASSIGNEE(S): Toray Industries, Inc., Japan

SOURCE: PCT Int. Appl., 146 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

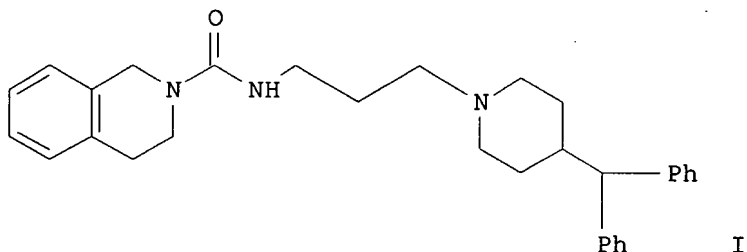
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002026708	A1	20020404	WO 2001-JP8466	20010927
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM			
RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
JP 2002187880	A	20020705	JP 2001-293350	20010926
AU 2001092276	A5	20020408	AU 2001-92276	20010927
PRIORITY APPLN. INFO.:			JP 2000-294355	A 20000927

OTHER SOURCE(S):
GI

MARPAT 136:294857



AB Title compds. [Ar(CH₂)_nA(CH₂)_m(Y)_xBB1; Ar = (un)substituted-1,2,3,4-tetrahydroisoquinoline-2-yl, 3-substituted-pyrimidine-2-one-1-yl, C₆H₅CH₂NHCH₂CH₂NH, 3-benzyl-imidazole-2-one-1-yl, 1,3-dihydro-isoindole-2-yl, C₆H₅, CONH(CH₂)₃; C(NH)NH(CH₂)₃, CO, N(CH₃)C(:NH)NH(CH₂)₃, N(CH₃)C(:NH)NHCH₂CH₂, n = 0, 1, 2, 3; A = 1-piperidinyl, 1-piperazinyl, 1-homopiperazinyl; m = 0, 1, 2, 3; x = 0, 1; Y = CO, SO₂; B = H, (un)substituted-aryl, (un)substituted-heterocyclyl; B1 = (un)substituted-aryl, electron pair, etc] and pharmaceutically acceptable salts are prepared and are useful as CCR3 inhibitors to be used in preventing and treating allergic inflammatory diseases caused by leukergy of lymphocytes, eosinocytes, basophilic leukocytes. Thus, the title compound I was prepared with 54% yield from 1,2,3,4-tetrahydroisoquinoline-2-carbonyl chloride and 3-(4-(diphenylmethyl)piperidinyl)propylamine in THF at room temperature for 4 h. The title compound I was tested for CCR3

inhibition

(IC₅₀ = 2.1 μM) with B300-19 cells.

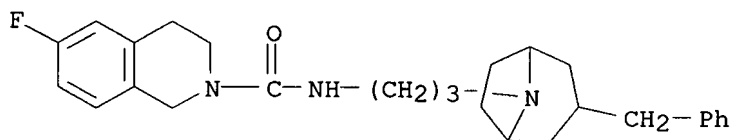
IT 406923-49-7P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of nitrogen-containing compds. as the active ingredient of CCR3 inhibitors)

RN 406923-49-7 CAPLUS

CN 2(1H)-Isoquinolinecarboxamide, 6-fluoro-3,4-dihydro-N-[3-[3-(phenylmethyl)-8-azabicyclo[3.2.1]oct-8-yl]propyl]- (9CI) (CA INDEX NAME)



REFERENCE COUNT:

23

THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 14 OF 28 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2001:749720 CAPLUS

DOCUMENT NUMBER: 136:37802

TITLE: Synthesis and biological evaluation of tropane-like 1-{2-[bis(4-fluorophenyl)methoxy]ethyl}-4-(3-phenylpropyl)piperazine (GBR 12909) analogs

AUTHOR(S): Zhang, Ying; Joseph, David B.; Bowen, Wayne D.;
 Flippen-Anderson, Judith L.; Dersch, Christina M.;
 Rothman, Richard B.; Jacobson, Arthur E.; Rice, Kenner
 C.
 CORPORATE SOURCE: Laboratory of Medicinal Chemistry National Institute
 of Diabetes and Digestive and Kidney Diseases,
 National Institutes of Health, Bethesda, MD,
 20892-0815, USA
 SOURCE: Journal of Medicinal Chemistry (2001), 44(23),
 3937-3945
 CODEN: JMCMAR; ISSN: 0022-2623
 PUBLISHER: American Chemical Society
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 136:37802

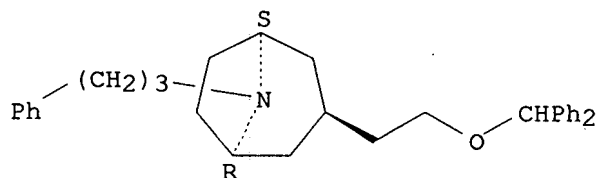
AB The authors have prepared azabicyclo[3.2.1] derivs. (C-3-substituted
 tropanes) that bind with high affinity to the dopamine transporter and
 inhibit dopamine reuptake. Within the series, 3-[2-[bis-(4-
 fluorophenyl)methoxy]ethylidene]-8-methyl-8-azabicyclo[3.2.1]octane (I)
 was found to have the highest affinity and selectivity for the dopamine
 transporter. These azabicyclo[3.2.1] (bridged piperidine) series of
 compds. differ from the well-known benztropines by a 2-carbon spacer
 between C-3 and a diarylmethoxy moiety. Interestingly, these new compds.
 demonstrated a much lower affinity for the muscarinic-1 site, at least a
 100-fold decrease compared to benztropine. Interestingly, these new
 compds. demonstrated a much lower affinity for the muscarinic-1 site, at
 least a 100-fold decrease compared to benztropine. Replacing N-Me with
 N-phenylpropyl in two of the compds. resulted in a 3-10-fold increase in
 binding affinity for the dopamine transporter. However, those compds.
 lost selectivity for the dopamine transporter over the serotonin
 transporter. Replacement of the ether oxygen in the diarylmethoxy moiety
 with a nitrogen atom gave relatively inactive amines, indicating the
 important role which is played by the ether oxygen in transporter binding.
 Reduction of the C-3 double bond in I gave 3 α -substituted tropanes, as
 shown by X-ray crystallog. analyses. The 3 α -substituted tropanes
 had lower affinity and less selectivity than the comparable unsatd.
 ligands.

IT 380602-02-8P 380602-03-9P
 RL: DMA (Drug mechanism of action); PAC (Pharmacological activity); SPN
 (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
 (preparation, muscarinic M1 receptor, dopamine and serotonin transporter
 affinity, and structure-activity relationship of azabicyclooctane
 derivs. as GBR 12909 analogs)

RN 380602-02-8 CAPLUS

CN 8-Azabicyclo[3.2.1]octane, 3-[2-(diphenylmethoxy)ethyl]-8-(3-phenylpropyl)-
 , hydrochloride, (3-endo)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



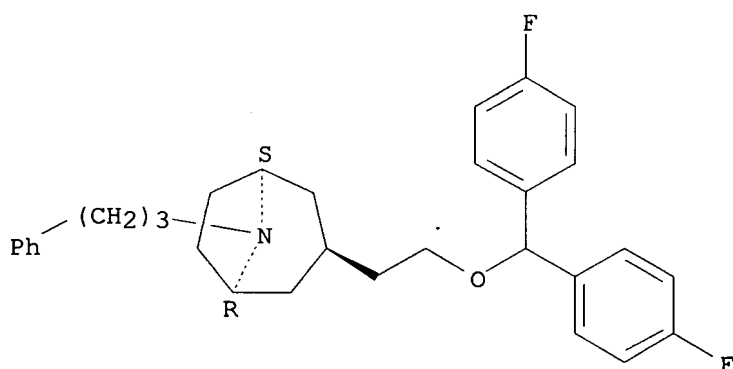
● HCl

RN 380602-03-9 CAPLUS

CN 8-Azabicyclo[3.2.1]octane, 3-[2-[bis(4-fluorophenyl)methoxy]ethyl]-8-(3-

phenylpropyl)-, hydrochloride, (3-endo)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



● HCl

REFERENCE COUNT: 42 THERE ARE 42 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 15 OF 28 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2001:338355 CAPLUS

DOCUMENT NUMBER: 134:340509

TITLE: Preparation of 8-azabicyclo[3.2.1]octane NMDA/NR2B antagonists

INVENTOR(S): Thompson, Wayne; Claremon, David A.; Munson, Peter M.; Phillips, Brian

PATENT ASSIGNEE(S): Merck & Co., Inc., USA

SOURCE: PCT Int. Appl., 77 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

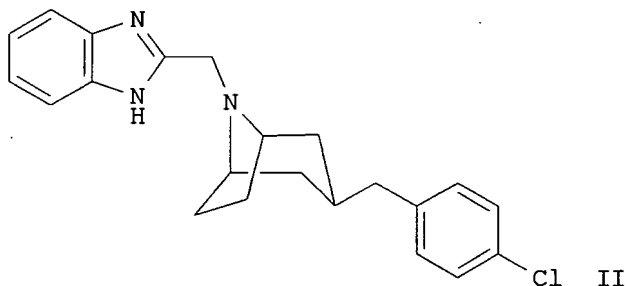
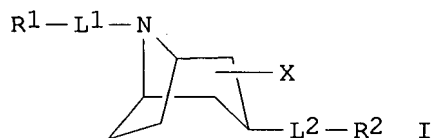
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001032179	A1	20010510	WO 2000-US29479	20001026
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM			
RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG			
US 6432976	B1	20020813	US 2000-696503	20001025
CA 2388171	A1	20010510	CA 2000-2388171	20001026
EP 1244450	A1	20021002	EP 2000-979131	20001026
R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL			
JP 2003513044	T	20030408	JP 2001-534384	20001026
PRIORITY APPLN. INFO.:			US 1999-162718P	P 19991029
			WO 2000-US29479	W 20001026

OTHER SOURCE(S): MARPAT 134:340509

GI



AB The title compds., commonly known as tropanes, (I) [wherein R1 = (un)substituted 2-benzimidazole, imidazole, imidazopyridine, indole, quinazoline, purine, benzoxazolone, or phenol; R2 = Ph, optionally substituted with 1-5 substituents selected from Cl, F, Br, alkyl, CF3, OH, or CO2H; L1 and L2 = independently (cyclo)alkyl, alkenyl, alkynyl, alkoxy, aminoalkyl, hydroxyalkyl, or (amino)carbonyl; X = OH, NH2, (di)alkylamino, alkyl, ester, carbamate, carbonate, or ether] were prepared as effective NMDA NR2B glutamate receptor antagonists. For example, addition of di-Et 4-chlorobenzylphosphonate to N-carbethoxy-4-tropinone to give the benzylidene, reduction using Pt/C, N-deprotection using HBr in AcOH, and reductive addition of 1-(trimethylsilylethoxymethyl)-1H-benzimidazole-2-carbaldehyde (2-step preparation given) using NaBH(OAc)3 in ClCH2CH2Cl afforded exo-II. Exptl. protocols for assessing the inhibition of NR1A/2B NMDA receptor activation (FLIPR assay) and determining the apparent dissociation consts.

against the human NR1A/NR2B receptor (binding assay) are given (no data). I are useful for relieving pain and treating migraine, depression, anxiety, schizophrenia, Parkinson's disease, or stroke (no data).

IT 338733-30-5P 338733-34-9P 338733-35-0P
338733-37-2P

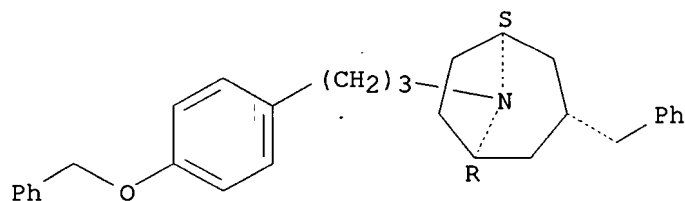
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(intermediate; preparation of (benzimidazolylalkyl)tropane NMDA/NR2B antagonists for treatment of pain)

RN 338733-30-5 CAPLUS

CN 8-Azabicyclo[3.2.1]octane, 8-[3-[4-(phenylmethoxy)phenyl]propyl]-3-(phenylmethyl)-, (3-exo)- (9CI) (CA INDEX NAME)

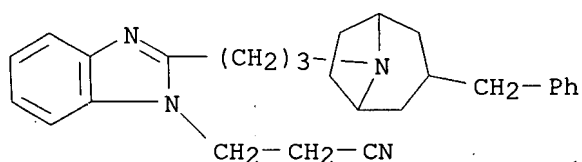
Relative stereochemistry.



RN 338733-34-9 CAPLUS

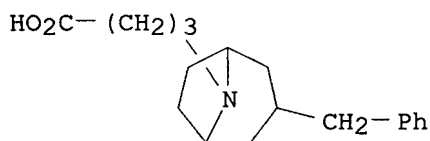
CN 1H-Benzimidazole-1-propanenitrile, 2-[3-[3-(phenylmethyl)-8-

azabicyclo[3.2.1]oct-8-yl]propyl]- (9CI) (CA INDEX NAME)



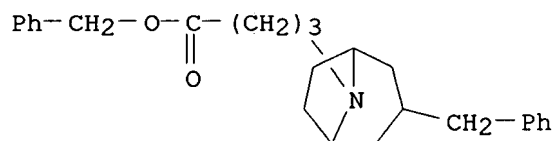
RN 338733-35-0 CAPLUS

CN 8-Azabicyclo[3.2.1]octane-8-butanoic acid, 3-(phenylmethyl)- (9CI) (CA INDEX NAME)



RN 338733-37-2 CAPLUS

CN 8-Azabicyclo[3.2.1]octane-8-butanoic acid, 3-(phenylmethyl)-, phenylmethyl ester (9CI) (CA INDEX NAME)



IT 338732-79-9P 338732-81-3P 338732-86-8P

338732-89-1P 338732-91-5P 338732-92-6P

338733-09-8P 338733-10-1P 338733-13-4P

338733-16-7P 338795-47-4P

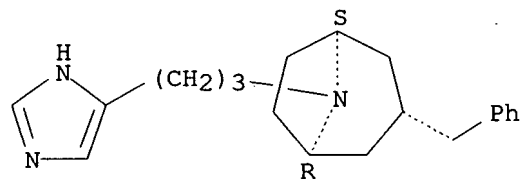
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of (benzimidazolylalkyl)tropane NMDA/NR2B antagonists for treatment of pain)

RN 338732-79-9 CAPLUS

CN 8-Azabicyclo[3.2.1]octane, 8-[3-(1H-imidazol-4-yl)propyl]-3-(phenylmethyl)-, (3-exo)- (9CI) (CA INDEX NAME)

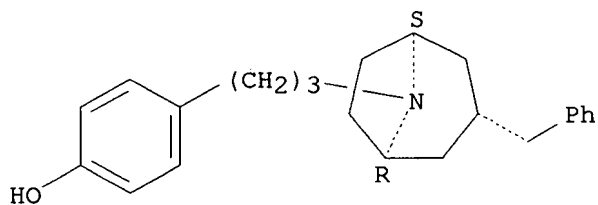
Relative stereochemistry.



RN 338732-81-3 CAPLUS

CN Phenol, 4-[3-[(3-exo)-3-(phenylmethyl)-8-azabicyclo[3.2.1]oct-8-yl]propyl]- (9CI) (CA INDEX NAME)

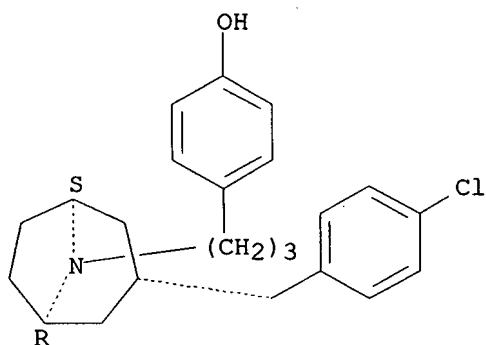
Relative stereochemistry.



RN 338732-86-8 CAPLUS

CN Phenol, 4-[3-[(3-exo)-3-[(4-chlorophenyl)methyl]-8-azabicyclo[3.2.1]oct-8-yl]propyl]- (9CI) (CA INDEX NAME)

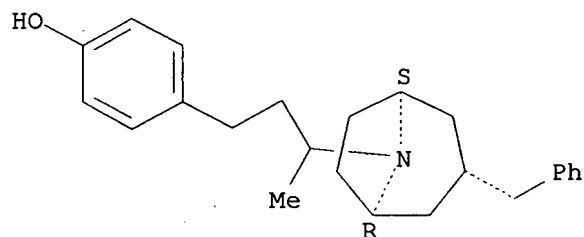
Relative stereochemistry.



RN 338732-89-1 CAPLUS

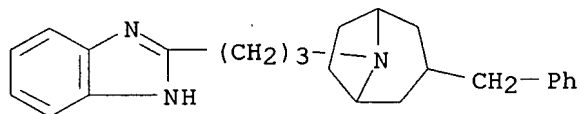
CN Phenol, 4-[3-[(3-exo)-3-(phenylmethyl)-8-azabicyclo[3.2.1]oct-8-yl]butyl]- (9CI) (CA INDEX NAME)

Relative stereochemistry.



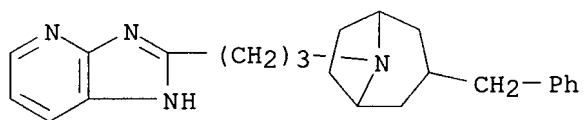
RN 338732-91-5 CAPLUS

CN 8-Azabicyclo[3.2.1]octane, 8-[3-(1H-benzimidazol-2-yl)propyl]-3-(phenylmethyl)- (9CI) (CA INDEX NAME)



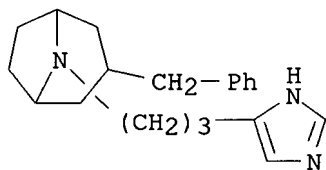
RN 338732-92-6 CAPLUS

CN 8-Azabicyclo[3.2.1]octane, 8-[3-(1H-imidazo[4,5-b]pyridin-2-yl)propyl]-3-(phenylmethyl)- (9CI) (CA INDEX NAME)



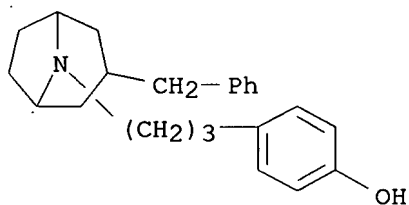
RN 338733-09-8 CAPLUS

CN 8-Azabicyclo[3.2.1]octane, 8-[3-(1H-imidazol-4-yl)propyl]-3-(phenylmethyl)-
(9CI) (CA INDEX NAME)



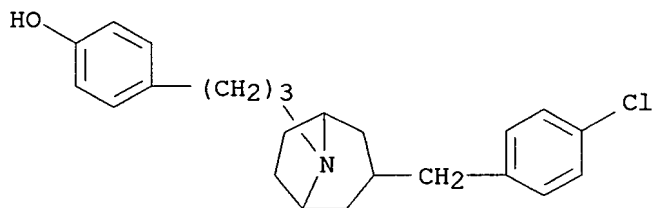
RN 338733-10-1 CAPLUS

CN Phenol, 4-[3-[3-(phenylmethyl)-8-azabicyclo[3.2.1]oct-8-yl]propyl]- (9CI)
(CA INDEX NAME)



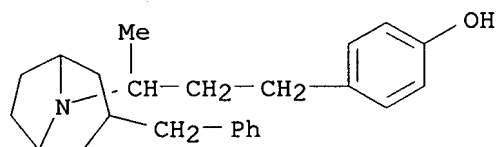
RN 338733-13-4 CAPLUS

CN Phenol, 4-[3-[3-[(4-chlorophenyl)methyl]-8-azabicyclo[3.2.1]oct-8-yl]propyl]- (9CI) (CA INDEX NAME)



RN 338733-16-7 CAPLUS

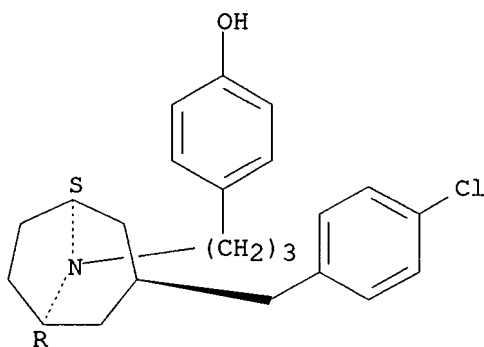
CN Phenol, 4-[3-[3-(phenylmethyl)-8-azabicyclo[3.2.1]oct-8-yl]butyl]- (9CI)
(CA INDEX NAME)



RN 338795-47-4 CAPLUS

CN Phenol, 4-[3-[(3-endo)-3-[(4-chlorophenyl)methyl]-8-azabicyclo[3.2.1]oct-8-yl]propyl]- (9CI) (CA INDEX NAME)

Relative stereochemistry.



REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 16 OF 28 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1998:402440 CAPLUS

DOCUMENT NUMBER: 129:67708

TITLE: Preparation of 8-azabicyclo[3.2.1]octane, 8-azabicyclo[3.2.1]oct-6-ene, 9-azabicyclo[3.3.1]nonane, 9-aza-3-oxabicyclo[3.3.1]nonane, and 9-aza-3-thiabicyclo[3.3.1]nonane derivatives as insecticides

INVENTOR(S): Urch, Christopher John; Lewis, Terence; Sunley, Raymond Leo; Salmon, Raymond; Godfrey, Christopher Richard Ayles; Brightwell, Christopher Ian; et al.

PATENT ASSIGNEE(S): Zeneca Ltd., UK

SOURCE: PCT Int. Appl., 65 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

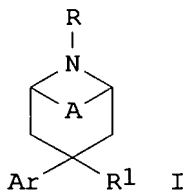
LANGUAGE: English

FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9825924	A1	19980618	WO 1997-GB3054	19971106
W:	AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW			
RW:	GH, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG			
ZA 9709840	A	19980526	ZA 1997-9840	19971031
CA 2271749	A1	19980618	CA 1997-2271749	19971106
AU 9748761	A	19980703	AU 1997-48761	19971106
AU 719147	B2	20000504		
EP 944627	A1	19990929	EP 1997-911349	19971106
EP 944627	B1	20040218		
R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI			
BR 9713136	A	20000208	BR 1997-13136	19971106
CN 1245499	A	20000223	CN 1997-181520	19971106
SI 20020	A	20000229	SI 1997-20086	19971106
HU 200000582	A2	20000628	HU 2000-582	19971106
JP 2001506989	T	20010529	JP 1998-526332	19971106

AT 259806	T	20040315	AT 1997-911349	19971106
ES 2216131	T3	20041016	ES 1997-911349	19971106
US 5968947	A	19991019	US 1997-969978	19971113
EG 21556	A	20011231	EG 1997-1269	19971126
US 6174894	B1	20010116	US 1999-357749	19990721
US 6177442	B1	20010123	US 1999-357750	19990721
US 6291474	B1	20010918	US 2000-635879	20000810
US 2002061913	A1	20020523	US 2001-886495	20010622
PRIORITY APPLN. INFO.:			GB 1996-24516	A 19961126
			GB 1996-24611	A 19961126
			GB 1996-24614	A 19961126
			WO 1997-GB3054	W 19971106
			US 1997-969639	A3 19971113
			US 1997-969978	A3 19971113
			US 1999-357750	A3 19990721
			US 2000-635879	A3 20000810
OTHER SOURCE(S):			MARPAT 129:67708	
GI				



AB Compds. of formula [I; A = a bidentate group of the formula CH_2XCH_2 (wherein X = methylene, O, or S), $\text{X}'\text{C:CY}$ or $\text{X}'\text{WCCYZ}$ (wherein X', W, Y, Z = H, OH, acyloxy, alkoxy, alkylsilyloxy, cyano or halogen, or X' and W or Y and Z together with the carbon to which they are attached form a carbonyl group), provided that $\text{A} \neq \text{CH}_2\text{CH}_2$; Ar = optionally substituted Ph or 5- or 6-membered heterocyclic ring system containing from 1 to 3 heteroatoms individually selected from N, O and S atoms, and at least one unsatn. (double bond) between adjacent atoms in the ring, said heterocyclic ring being optionally fused to a benzene ring; R = H or cyano or a group selected from alkyl, aryl, heteroaryl, aralkyl, heteroarylalkyl, alkenyl, aralkenyl, alkynyl, alkoxycarbonyl, alkanesulfonyl, arenesulfonyl, alkenyloxycarbonyl, aralkyloxycarbonyl, aryloxycarbonyl, heterocyclylalkyl, carbamoyl, dithiocarboxyl, etc.; R1 = H, cyano, HO, alkyl, alkoxy, NH_2 , NO_2 , isocyanato, acylamino, hydroxyalkyl, optionally substituted heteroaryl, alkoxyalkyl, haloalkyl, halohydroxyalkyl, etc.; alkyl moieties of R comprise from 1 to 15 carbon atoms, and are optionally substituted with one or more substituents selected from, halogen, cyano, carboxyl, carboxyl acyl, etc.] or an acid addition salt, quaternary ammonium salt or N-oxide derived therefrom are prepared Also claimed are an insecticidal, acaricidal or nematocidal composition comprising a compound of formula I and a suitable carrier or diluent therefor and a method of combating and controlling insect, acarid or nematode pests at a locus which comprises treating the pests or the locus of the pests with an effective amount of a compound of formula I or a composition as hereinbefore described. Thus, *exo*-3-cyano-9-methyl-9-azabicyclo[3.3.1]nonane and 3,5-dichloropyridine (preparation given) in THF were treated dropwise with lithium bis(trimethylsilyl)amide, and the reaction mixture was allowed to react ambient temperature for 18 h to give I [A = $(\text{CH}_2)_3$, Ar = *exo*-5-chloropyridyl, R = Me, R1 = *endo*-cyano], which at 500 ppm showed 80-100% mortality against peach aphid (*Myzus persicae*).

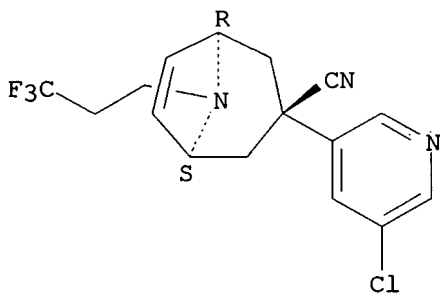
IT 209054-33-1P 209054-36-4P
 RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic

preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of azabicyclo[3.2.1]octane, azabicyclo[3.2.1]octene,
azabicyclo[3.3.1]nonane, azaoxabicyclo[3.3.1]nonane, and
azathiabicyclo[3.3.1]nonane derivs. as insecticides, nematocides, and
acaricides)

RN 209054-33-1 CAPLUS

CN 8-Azabicyclo[3.2.1]oct-6-ene-3-carbonitrile, 3-(5-chloro-3-pyridinyl)-8-
(3,3,3-trifluoropropyl)-, (3-endo)- (9CI) (CA INDEX NAME)

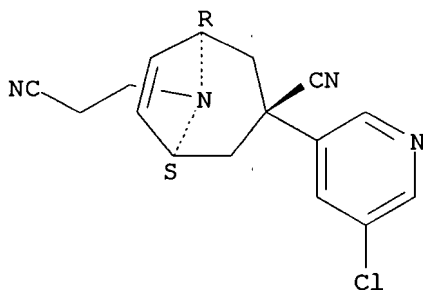
Relative stereochemistry.



RN 209054-36-4 CAPLUS

CN 8-Azabicyclo[3.2.1]oct-6-ene-8-propanenitrile, 3-(5-chloro-3-pyridinyl)-3-
cyano-, (3-endo)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



REFERENCE COUNT: 13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 17 OF 28 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1997:330897 CAPLUS

DOCUMENT NUMBER: 127:44445

TITLE: The SAR of UK-78,282: a novel blocker of human T cell
Kv1.3 potassium channels

AUTHOR(S): Burgess, Laurence E.; Koch, Kevin; Cooper, Kelvin;
Biggers, Michael S.; Ramchandani, Mukesh; Smitrovich,
Jacqueline H.; Gilbert, Eric J.; Bruns, Matthew J.;
Mather, Robert J.; et al.

CORPORATE SOURCE: Central Research Division, Department of Medicinal
Chemistry, Pfizer Inc., Groton, CT, 06340, USA

SOURCE: Bioorganic & Medicinal Chemistry Letters (1997), 7(8),
1047-1052

CODEN: BMCLE8; ISSN: 0960-894X

PUBLISHER: Elsevier

DOCUMENT TYPE: Journal

LANGUAGE: English

AB UK-78,282 was identified in a human T cell 86Rb efflux high-throughput
screen of our compound libraries. This compound was found to be a potent and

selective blocker of human T cell voltage-gated K⁺ channels and to inhibit T cell activation. The SAR around UK-78,282 and a general pharmacophore hypothesis are presented in this communication.

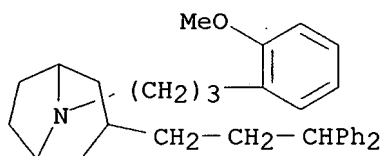
IT 191217-58-0

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)

(structure-activity relationships of synthetic derivs. of UK-78,282 T-cell Kv1.3 potassium channel blocker)

RN 191217-58-0 CAPLUS

CN 8-Azabicyclo[3.2.1]octane, 3-(3,3-diphenylpropyl)-8-[3-(2-methoxyphenyl)propyl]- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 30 THERE ARE 30 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 18 OF 28 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1997:101571 CAPLUS

DOCUMENT NUMBER: 126:104021

TITLE: Preparation of 3-aryl-3-cyano-8-azabicyclo[3.2.1]octanes as insecticides and acaricides.

INVENTOR(S): Urch, Christopher John; Salmon, Roger; Lewis, Terence; Godfrey, Christopher Richard Ayles; Clough, Martin Stephen

PATENT ASSIGNEE(S): Zeneca Limited, UK

SOURCE: PCT Int. Appl., 77 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

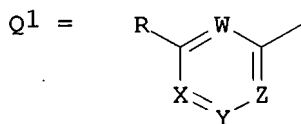
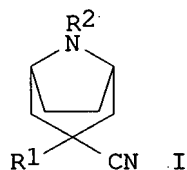
FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9637494	A1	19961128	WO 1996-GB1151	19960513
W: AL, AM, AT, AU, AZ, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IS, JP, KE, KG, KP, KR, KZ, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI				
RW: KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN				
CA 2217064	A1	19961128	CA 1996-2217064	19960513
AU 9656988	A	19961211	AU 1996-56988	19960513
AU 710540	B2	19990923		
EP 828739	A1	19980318	EP 1996-915100	19960513
EP 828739	B1	20020911		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI				
CN 1185154	A	19980617	CN 1996-194135	19960513
CN 1066730	B	20010606		
GB 2324795	A	19981104	GB 1998-16362	19960513
GB 2324795	B	19990519		
HU 9802708	A2	19990201	HU 1998-2708	19960513
BR 9609112	A	19990202	BR 1996-9112	19960513

JP 11505826	T	19990525	JP 1996-535466	19960513
AP 803	A	20000124	AP 1997-1139	19960513
W: GH, KE, LS, MW, SD, SZ, UG, ZW				
AT 223913	T	20020915	AT 1996-915100	19960513
PT 828739	T	20021231	PT 1996-915100	19960513
ES 2183950	T3	20030401	ES 1996-915100	19960513
IL 118254	A	20020421	IL 1996-118254	19960514
IL 127075	A	20030212	IL 1996-127075	19960514
ZA 9603875	A	19961202	ZA 1996-3875	19960515
IN 1996DE01041	A	20050311	IN 1996-DE1041	19960517
US 5922732	A	19990713	US 1996-651182	19960524
US 6207676	B1	20010327	US 1998-207195	19981208
AU 9936832	A	19990916	AU 1999-36832	19990629
AU 720176	B2	20000525		
US 6391883	B1	20020521	US 2000-602711	20000626
US 6573275	B1	20030603	US 2002-124696	20020412
PRIORITY APPLN. INFO.:			GB 1995-10459	A 19950524
			AU 1996-56988	A3 19960513
			GB 1996-9978	A3 19960513
			WO 1996-GB1151	W 19960513
			IL 1996-118254	A3 19960514
			US 1996-651182	A3 19960524
			US 1998-207195	A3 19981208
			US 2000-602711	A3 20000626

OTHER SOURCE(S): MARPAT 126:104021
GI



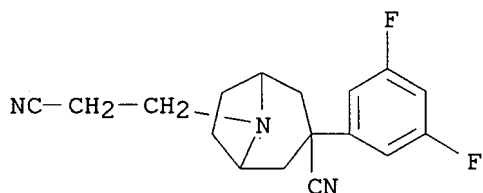
AB Title compds. [I; R1 = Q1; W, X, Y, Z = CR, N; provided that ≤ 2 of W, X, Y, Z = N; R = H, halo, cyano, amino, hydrazino, acylamino, OH, alkyl, hydroxyalkyl, alkoxy, haloalkyl, haloalkoxy, alkenyl, alkenyloxy, alkoxyalkenyl, alkynyl, carboxylic acyl, alkoxy carbonyl, aryl, heterocyclyl; R2 = H, cyano, (substituted) alkyl, aryl, heteroaryl, aralkyl, heteroarylalkyl, alkenyl, aralkenyl, alkynyl, alkoxy carbonyl, alkanesulfonyl, arenesulfonyl, alkanyloxy carbonyl, aralkyloxy carbonyl, arloxy carbonyl, heterocyclylalkyl, carbamyl, dithiocarboxyl], were prepared Thus, tropinone and tosylmethyl isocyanide in dimethoxyethane/EtOH at 0° were treated with KOCMe3 and the mixture was stirred 4 h at room temperature to give exo-3-cyano-8-methyl-8-azabicyclo[3.2.1]octane. The latter in THF was added to LiN(CHMe2)2 in THF at -25° and the mixture was cooled to -78°; 3-fluoropyridine was added and the mixture was warmed to room temperature over 6 h to give exo-3-(3-pyridyl)-endo-3-cyano-8-methyl-8-azabicyclo[3.2.1]octane. The latter at 500 ppm was 80-100% effective against *Myzus persicae*.

IT 185982-37-0P 185982-51-8P 185982-87-0P
185982-89-2P 185983-07-7P 185983-58-8P
185983-59-9P 185983-78-2P 185983-97-5P
185984-13-8P 185984-31-0P 185984-47-8P
185984-58-1P 185985-20-0P 185985-21-1P
185985-24-4P
RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of 3-aryl-3-cyano-8-azabicyclo[3.2.1]octanes as insecticides

and acaricides)

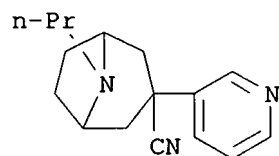
RN 185982-37-0 CAPLUS

CN 8-Azabicyclo[3.2.1]octane-8-propanenitrile, 3-cyano-3-(3,5-difluorophenyl)-
(9CI) (CA INDEX NAME)



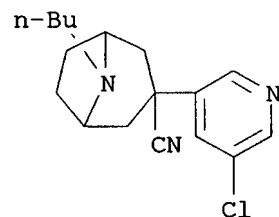
RN 185982-51-8 CAPLUS

CN 8-Azabicyclo[3.2.1]octane-3-carbonitrile, 8-propyl-3-(3-pyridinyl)- (9CI)
(CA INDEX NAME)



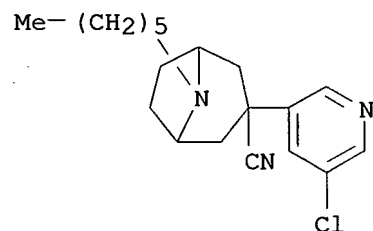
RN 185982-87-0 CAPLUS

CN 8-Azabicyclo[3.2.1]octane-3-carbonitrile, 8-butyl-3-(5-chloro-3-pyridinyl)-
(9CI) (CA INDEX NAME)



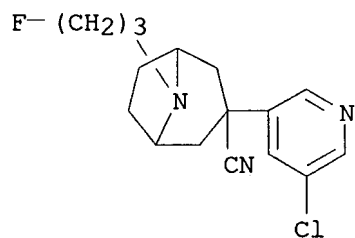
RN 185982-89-2 CAPLUS

CN 8-Azabicyclo[3.2.1]octane-3-carbonitrile, 3-(5-chloro-3-pyridinyl)-8-hexyl-
(9CI) (CA INDEX NAME)



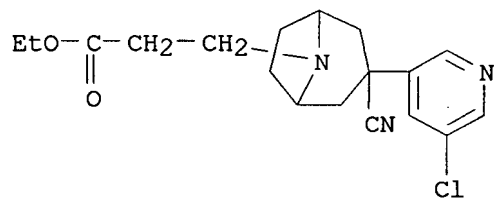
RN 185983-07-7 CAPLUS

CN 8-Azabicyclo[3.2.1]octane-3-carbonitrile, 3-(5-chloro-3-pyridinyl)-8-(3-fluoropropyl)- (9CI) (CA INDEX NAME)



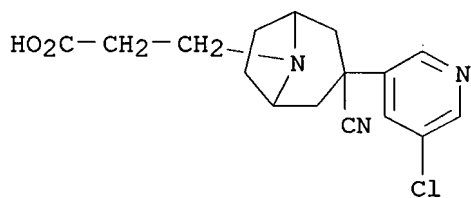
RN 185983-58-8 CAPLUS

CN 8-Azabicyclo[3.2.1]octane-8-propanoic acid, 3-(5-chloro-3-pyridinyl)-3-cyano-, ethyl ester (9CI) (CA INDEX NAME)



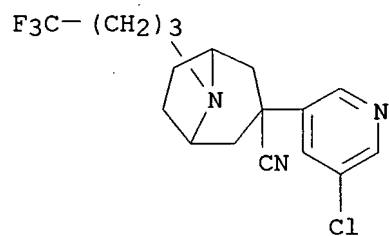
RN 185983-59-9 CAPLUS

CN 8-Azabicyclo[3.2.1]octane-8-propanoic acid, 3-(5-chloro-3-pyridinyl)-3-cyano- (9CI) (CA INDEX NAME)



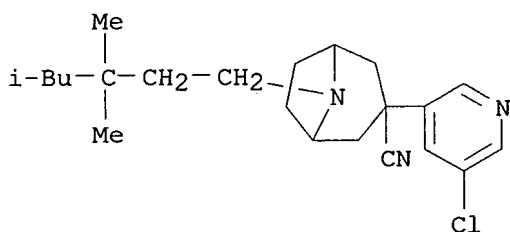
RN 185983-78-2 CAPLUS

CN 8-Azabicyclo[3.2.1]octane-3-carbonitrile, 3-(5-chloro-3-pyridinyl)-8-(4,4,4-trifluorobutyl)- (9CI) (CA INDEX NAME)



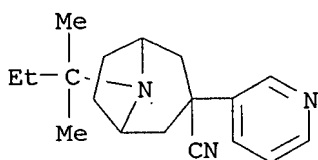
RN 185983-97-5 CAPLUS

CN 8-Azabicyclo[3.2.1]octane-3-carbonitrile, 3-(5-chloro-3-pyridinyl)-8-(3,3,5-trimethylhexyl)- (9CI) (CA INDEX NAME)



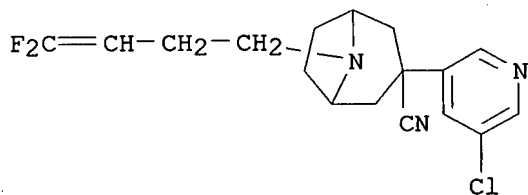
RN 185984-13-8 CAPLUS

CN 8-Azabicyclo[3.2.1]octane-3-carbonitrile, 8-(1,1-dimethylpropyl)-3-(3-pyridinyl)- (9CI) (CA INDEX NAME)



RN 185984-31-0 CAPLUS

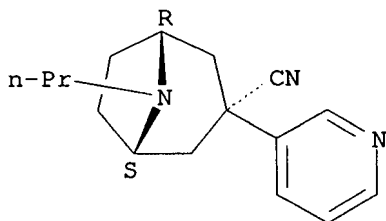
CN 8-Azabicyclo[3.2.1]octane-3-carbonitrile, 3-(5-chloro-3-pyridinyl)-8-(4,4-difluoro-3-butenyl)- (9CI) (CA INDEX NAME)



RN 185984-47-8 CAPLUS

CN 8-Azabicyclo[3.2.1]octane-3-carbonitrile, 8-propyl-3-(3-pyridinyl)-, endo- (9CI) (CA INDEX NAME)

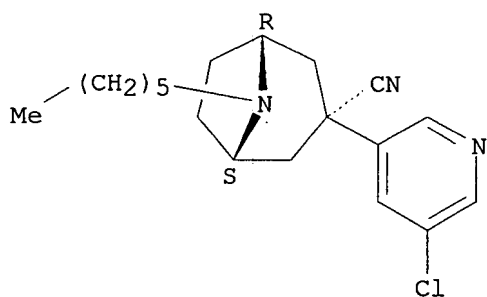
Relative stereochemistry.



RN 185984-58-1 CAPLUS

CN 8-Azabicyclo[3.2.1]octane-3-carbonitrile, 3-(5-chloro-3-pyridinyl)-8-hexyl-, endo- (9CI) (CA INDEX NAME)

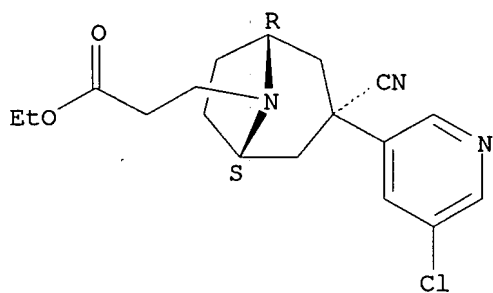
Relative stereochemistry.



RN 185985-20-0 CAPLUS

CN 8-Azabicyclo[3.2.1]octane-8-propanoic acid, 3-(5-chloro-3-pyridinyl)-3-cyano-, ethyl ester, endo- (9CI) (CA INDEX NAME)

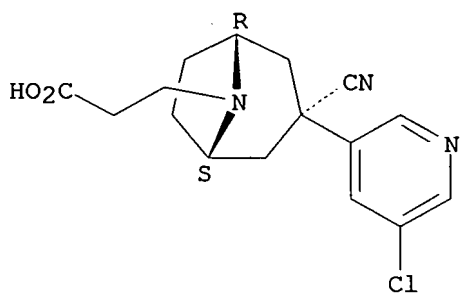
Relative stereochemistry.



RN 185985-21-1 CAPLUS

CN 8-Azabicyclo[3.2.1]octane-8-propanoic acid, 3-(5-chloro-3-pyridinyl)-3-cyano-, endo- (9CI) (CA INDEX NAME)

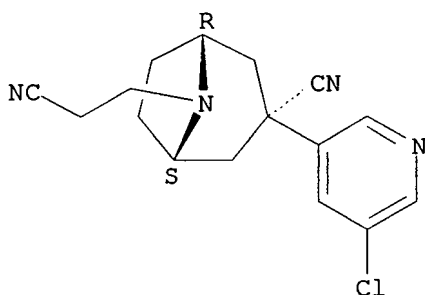
Relative stereochemistry.



RN 185985-24-4 CAPLUS

CN 8-Azabicyclo[3.2.1]octane-8-propanenitrile, 3-(5-chloro-3-pyridinyl)-3-cyano-, endo- (9CI) (CA INDEX NAME)

Relative stereochemistry.



L4 ANSWER 19 OF 28 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1994:106776 CAPLUS

DOCUMENT NUMBER: 120:106776

TITLE: Preparation of (phenoxyalkyl)piperidines and analogs as calcium channel antagonists

INVENTOR(S): Brown, Thomas Henry; Cooper, David Gwyn; King, Ronald Joseph; Orlek, Barry Sidney

PATENT ASSIGNEE(S): SmithKline Beckman Corp., UK

SOURCE: PCT Int. Appl., 56 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

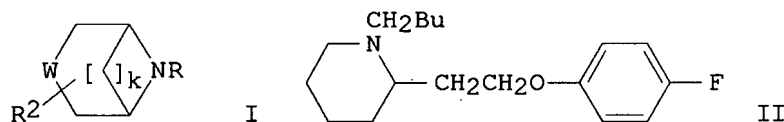
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9315052	A1	19930805	WO 1993-GB173	19930127
W: AU, CA, JP, KR, NZ, US				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
AU 9333644	A	19930901	AU 1993-33644	19930127
EP 629190	A1	19941221	EP 1993-902469	19930127
R: BE, CH, DE, FR, GB, IT, LI, NL				
JP 07503461	T	19950413	JP 1993-513047	19930127
PRIORITY APPLN. INFO.:				
			GB 1992-1744	A 19920128
			GB 1992-1745	A 19920128
			GB 1992-1746	A 19920128
			GB 1992-1752	A 19920128
			WO 1993-GB173	A 19930127

OTHER SOURCE(S): MARPAT 120:106776

GI



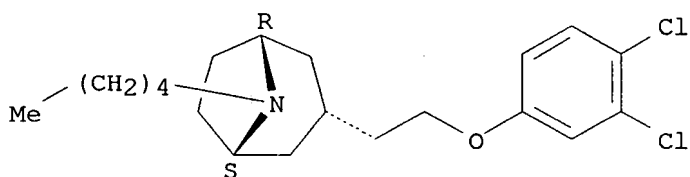
AB Title compds. [I; R = H (k = 2), (cyclo)alkyl, phenylalkyl, etc.; R2 = (CH2)nA(CH2)mR3; A = bond, CH:CH, O, NH, etc.; R3 = (hetero)aryl; W = bond, CH2, O, S; k = 0 or 2 when W = CH2; m, n = 0-6] were prepared. Thus, 2-(2-hydroxyethyl)piperidine was N-alkylated by BuCH2Br and the product condensed with 4-FC6H4OH to give title compound II. I gave 30-100% inhibition of plateau Ca²⁺ current in rat dorsal root ganglion neurons at 20 μ M in vitro.

IT 152009-16-0P 152601-96-2P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of, as calcium channel antagonist)
 RN 152009-16-0 CAPLUS
 CN 8-Azabicyclo[3.2.1]octane, 3-[2-(3,4-dichlorophenoxy)ethyl]-8-pentyl-,
 endo- (9CI) (CA INDEX NAME)

Relative stereochemistry.

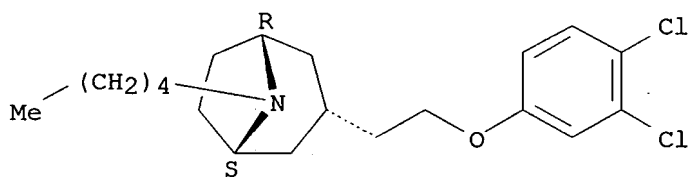


RN 152601-96-2 CAPLUS
 CN 8-Azabicyclo[3.2.1]octane, 3-[2-(3,4-dichlorophenoxy)ethyl]-8-pentyl-,
 endo-, ethanedioate (1:1) (9CI) (CA INDEX NAME)

CM 1

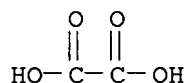
CRN 152009-16-0
 CMF C20 H29 Cl2 N O

Relative stereochemistry.



CM 2

CRN 144-62-7
 CMF C2 H2 O4



L4 ANSWER 20 OF 28 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1993:93788 CAPLUS

DOCUMENT NUMBER: 118:93788

TITLE: Opioid properties of some derivatives of pethidine based on tropane

AUTHOR(S): Casy, A. F.; Dewar, G. H.; Pascoe, R. A.

CORPORATE SOURCE: Sch. Pharm. Pharmacol., Univ. Bath, Bath, BA2 7AY, UK

SOURCE: Journal of Pharmacy and Pharmacology (1992), 44(10), 787-90

CODEN: JPPMAB; ISSN: 0022-3573

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 118:93788

AB The preparation of some tropane analogs of pethidine and its reversed ester, chiefly with preferred 3 α -m-hydroxyphenyl chair conformations, is described. The former were secured from tropan-3-one in a sequence of

reactions involving cyanide attack, hydrolysis, Grignard attack and then rearrangements. The reversed ester was obtained by treating tropan-3-one with lithium Ph, followed by acylation. Configurational and conformational assignments follow from NMR anal. The antinociceptive potencies of these compds. in mice are reported, and discussed in relation to non-phenolic congeners and the 4-arylpiperidine moiety of morphine.

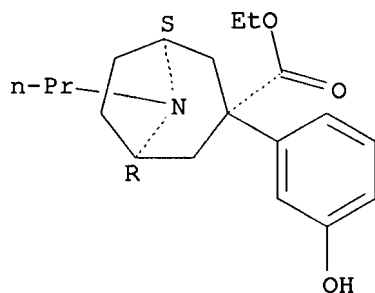
IT 145879-81-8P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation and analgesic activity of)

RN 145879-81-8 CAPLUS

CN 8-Azabicyclo[3.2.1]octane-3-carboxylic acid, 3-(3-hydroxyphenyl)-8-propyl-, ethyl ester, exo- (9CI) (CA INDEX NAME)

Relative stereochemistry.



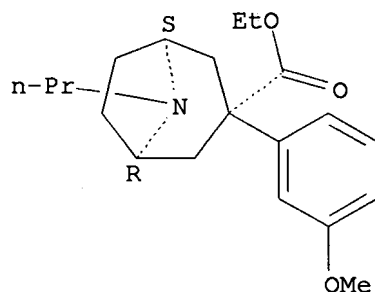
IT 145879-74-9P 145879-75-0P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 145879-74-9 CAPLUS

CN 8-Azabicyclo[3.2.1]octane-3-carboxylic acid, 3-(3-methoxyphenyl)-8-propyl-, ethyl ester, hydrochloride, exo- (9CI) (CA INDEX NAME)

Relative stereochemistry.

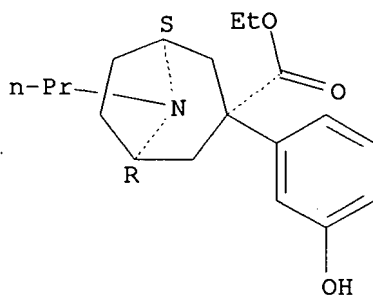


● HCl

RN 145879-75-0 CAPLUS

CN 8-Azabicyclo[3.2.1]octane-3-carboxylic acid, 3-(3-hydroxyphenyl)-8-propyl-, ethyl ester, hydrochloride, exo- (9CI) (CA INDEX NAME)

Relative stereochemistry.



● HCl

L4 ANSWER 21 OF 28 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1988:55866 CAPLUS

DOCUMENT NUMBER: 108:55866

TITLE: Synthesis and neuromuscular blocking activity of symmetrical bis- and poly-quaternary derivatives of quinuclidine and tropine

AUTHOR(S): Chen, Shengquan; Yu, Shongtao; Geng, Rongliang; Dan, Zhiyi

CORPORATE SOURCE: Inst. Basic Med. Sci., Acad. Mil. Med. Sci., Beijing, Peop. Rep. China

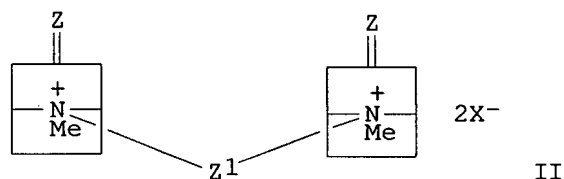
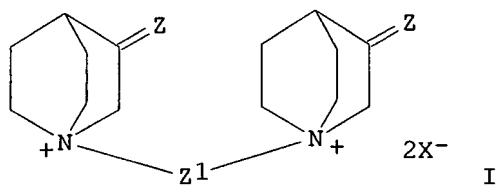
SOURCE: Yaoxue Xuebao (1987), 22(5), 347-53

CODEN: YHHPAL; ISSN: 0513-4870

DOCUMENT TYPE: Journal

LANGUAGE: Chinese

GI



AB Title compds. e.g., I and II [Z = O, NOH; Z1 = (CH2)6, CH2OCH2; X = Br, Cl] were prepared from quinuclidine or tropine derivs. and their neuromuscular blocking activity was reported.

IT 112546-62-0P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and neuromuscular blocking activity of)

RN 112546-62-0 CAPLUS

CN 8-Azoniabicyclo[3.2.1]octane, 8,8'-(1,6-hexanediyl)bis[3-(2-ethoxy-2-oxoethyl)-8-methyl-, dibromide (9CI) (CA INDEX NAME)

*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***

ACCESSION NUMBER: 1983:161003 CAPLUS

DOCUMENT NUMBER: 98:161003

TITLE: Tropyli derivatives

INVENTOR(S): Tomesch, John C.

PATENT ASSIGNEE(S): Sandoz, Inc., USA

SOURCE: U.S., 9 pp.

CODEN: USXXAM

DOCUMENT TYPE: Patent

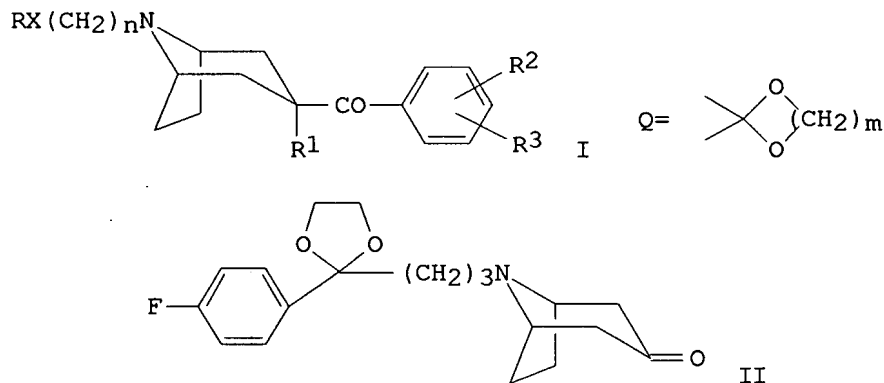
LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 4366154	A	19821228	US 1981-319254	19811109
PRIORITY APPLN. INFO.:			US 1981-319254	19811109
OTHER SOURCE(S):	CASREACT 98:161003; MARPAT 98:161003			

GI



AB The neurotropic (no data) title compds. I [R = (un)substituted Ph, (un)substituted 10H-phenothiazin-10-yl; R1 = H, HO; R2, R3 = H, F, Cl, Br, Cl-4 alkyl, Cl-4 alkoxy, F3C; n = 1-4; X = CO, Q (m = 2, 3)] and their salts were prepared. Thus, 2,6-cycloheptadienone cyclized with 2-(4-fluorophenyl)-1,3-dioxolane-2-propanamine to give the azabicyclooctanone II, which reacted with p-FC6H4CH(OEt)P(O)(OEt)2 followed by hydrolysis to give I (RX = p-FC6H4CO, R1 = R2 = H, R3 = p-F, n = 3).

IT 85329-99-3P 85330-00-3P

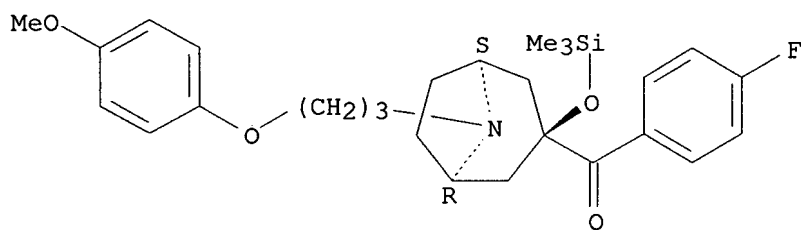
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and hydrolysis of)

RN 85329-99-3 CAPLUS

CN Methanone, (4-fluorophenyl)[8-[3-(4-methoxyphenoxy)propyl]-3-[(trimethylsilyl)oxy]-8-azabicyclo[3.2.1]oct-3-yl]-, endo- (9CI) (CA INDEX NAME)

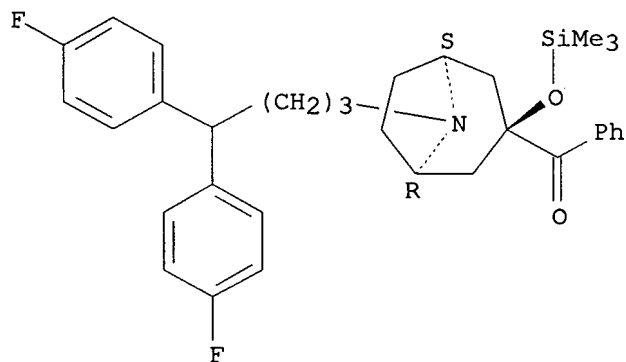
Relative stereochemistry.



RN 85330-00-3 CAPLUS

CN Methanone, [8-[4,4-bis(4-fluorophenyl)butyl]-3-[(trimethylsilyl)oxy]-8-azabicyclo[3.2.1]oct-3-yl]phenyl-, endo- (9CI) (CA INDEX NAME)

Relative stereochemistry.



IT 85329-92-6P 85329-97-1P 85329-98-2P

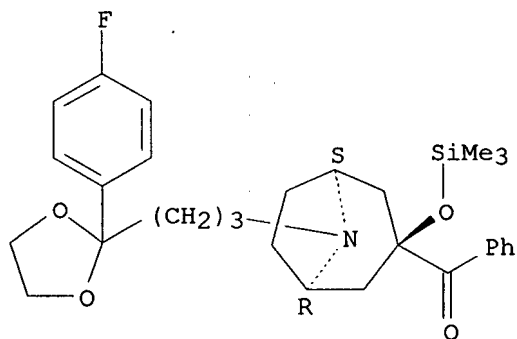
85330-02-5P 85330-04-7P 85345-63-7P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 85329-92-6 CAPLUS

CN Methanone, [8-[3-[2-(4-fluorophenyl)-1,3-dioxolan-2-yl]propyl]-3-[(trimethylsilyl)oxy]-8-azabicyclo[3.2.1]oct-3-yl]phenyl-, endo- (9CI)
(CA INDEX NAME)

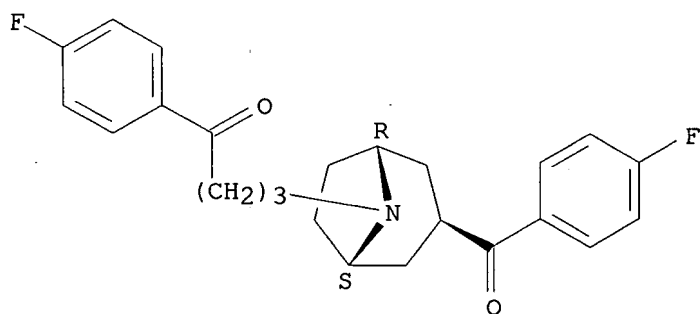
Relative stereochemistry.



RN 85329-97-1 CAPLUS

CN 1-Butanone, 4-[3-(4-fluorobenzoyl)-8-azabicyclo[3.2.1]oct-8-yl]-1-(4-fluorophenyl)-, exo- (9CI) (CA INDEX NAME)

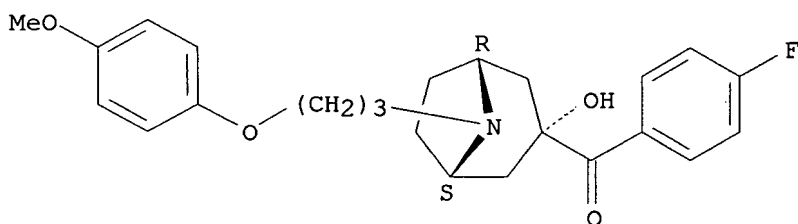
Relative stereochemistry.



RN 85329-98-2 CAPLUS

CN Methanone, (4-fluorophenyl)[3-hydroxy-8-[3-(4-methoxyphenoxy)propyl]-8-azabicyclo[3.2.1]oct-3-yl]-, endo- (9CI) (CA INDEX NAME)

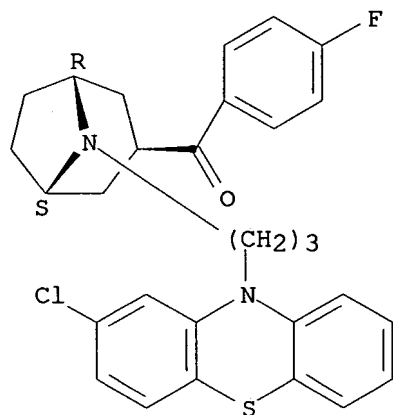
Relative stereochemistry.



RN 85330-02-5 CAPLUS

CN Methanone, [8-[3-(2-chloro-10H-phenothiazin-10-yl)propyl]-8-azabicyclo[3.2.1]oct-3-yl](4-fluorophenyl)-, exo- (9CI) (CA INDEX NAME)

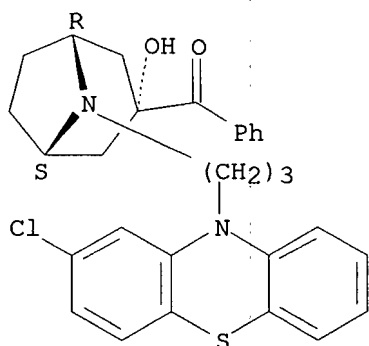
Relative stereochemistry.



RN 85330-04-7 CAPLUS

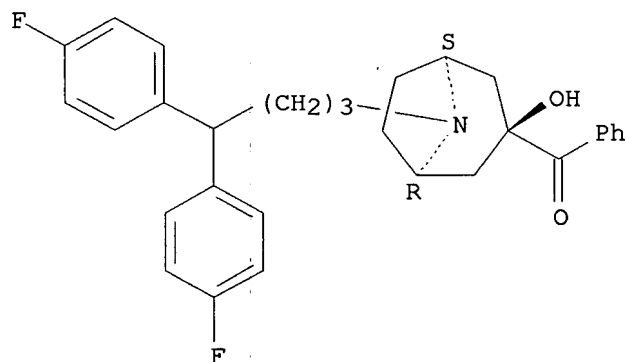
CN Methanone, [8-[3-(2-chloro-10H-phenothiazin-10-yl)propyl]-3-hydroxy-8-azabicyclo[3.2.1]oct-3-yl]phenyl-, endo- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 85345-63-7 CAPLUS
 CN Methanone, [8-[4,4-bis(4-fluorophenyl)butyl]-3-hydroxy-8-azabicyclo[3.2.1]oct-3-yl]phenyl-, endo- (9CI) (CA INDEX NAME)

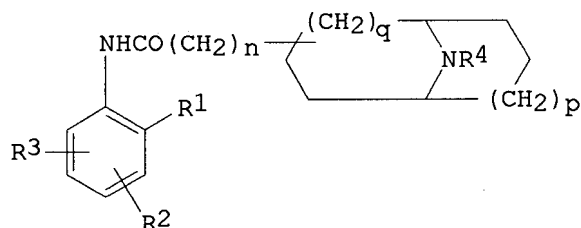
Relative stereochemistry.



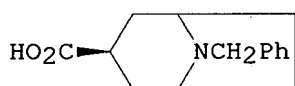
L4 ANSWER 23 OF 28 CAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 1982:6586 CAPLUS
 DOCUMENT NUMBER: 96:6586
 TITLE: Aniline derivatives
 INVENTOR(S): Hadley, Michael Stewart; Blaney, Frank Edward
 PATENT ASSIGNEE(S): Beecham Group Ltd. , UK
 SOURCE: Eur. Pat. Appl., 98 pp.
 CODEN: EPXXDW
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 31219	A1	19810701	EP 1980-304467	19801211
EP 31219	B1	19840307		
R: AT, BE, CH, DE, FR, GB, IT, NL, SE				
US 4350691	A	19820921	US 1980-213237	19801205
ZA 8007691	A	19811125	ZA 1980-7691	19801209
DK 8005414	A	19810621	DK 1980-5414	19801218
AU 8065528	A	19810625	AU 1980-65528	19801218
JP 56092888	A	19810727	JP 1980-180319	19801219
ES 498013	A1	19820401	ES 1980-498013	19801219
PRIORITY APPLN. INFO.:			GB 1979-43985	A 19791220
OTHER SOURCE(S):	MARPAT 96:6586			

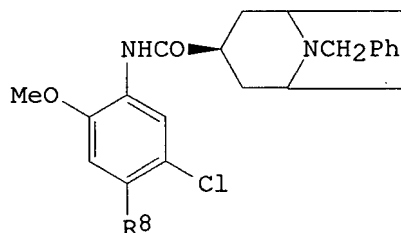
GI



I



II



III

AB Carboxamides I [R1 = C1-6 alkoxy or alkylthio; R2, R3 independently = H, halo, CF3, C1-7 acyl or acylamino, NH2, N2NCO, or H2NSO2 optionally substituted (o.s.) by 1 or 2 C1-6 alkyl, alkylsulfonyl, sulfinyl, thio, or alkoxy, OH, NO2; R1R2 = OCH2O, OCH2CH2O; R4 = C1-7 alkyl, (CH2)sR6 [s = 0-2, R6 = C3-8 cycloalkyl, (CH2)t R7 (t = 1, 2, R7 = Ph o.s. by 1 or 2 C1-6 alkyl, C1-4 alkoxy, CF3, halo, thienyl)], n, p, q independently = 0-2], useful as antiemetics, central nervous depressants, and gastric motility promoters, were prepared 8-Benzyl-nortropan-3-one was converted in 2 steps to bicyclic acid II which was successively amidated to amide III (R8 = H), nitrated to III (R8 = NO2), hydrogenated to amine III (R8 = NH2), and N-acylated to III (R8 = AcNH). III (R8 = NH2) had depressant ED50 0.05 mg/kg (mouse climbing test); 1 mg/kg gave 100% inhibition of climbing.

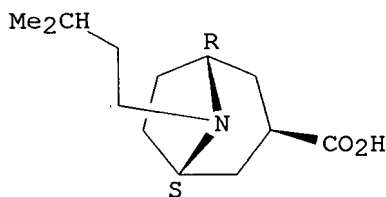
IT 79522-04-6

RL: RCT (Reactant); RACT (Reactant or reagent)
(amidation of, by aminochloroanizole)

RN 79522-04-6 CAPLUS

CN 8-Azabicyclo[3.2.1]octane-3-carboxylic acid, 8-(3-methylbutyl)-, hydrochloride, exo- (9CI) (CA INDEX NAME)

Relative stereochemistry.



● HCl

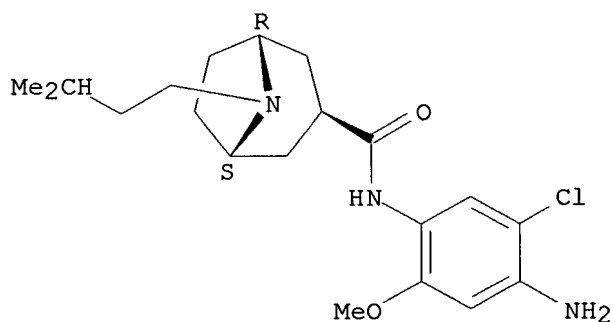
IT 79522-25-1P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation and depressant activity of)

RN 79522-25-1 CAPLUS

CN 8-Azabicyclo[3.2.1]octane-3-carboxamide, N-(4-amino-5-chloro-2-methoxyphenyl)-8-(3-methylbutyl)-, exo- (9CI) (CA INDEX NAME)

Relative stereochemistry.



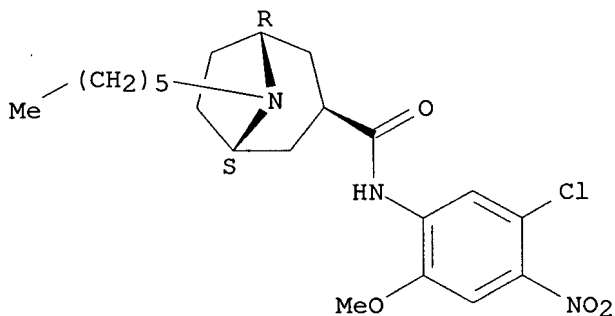
IT 79522-16-0P 79522-17-1P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and hydrogenation of)

RN 79522-16-0 CAPLUS

CN 8-Azabicyclo[3.2.1]octane-3-carboxamide, N-(5-chloro-2-methoxy-4-nitrophenyl)-8-hexyl-, exo- (9CI) (CA INDEX NAME)

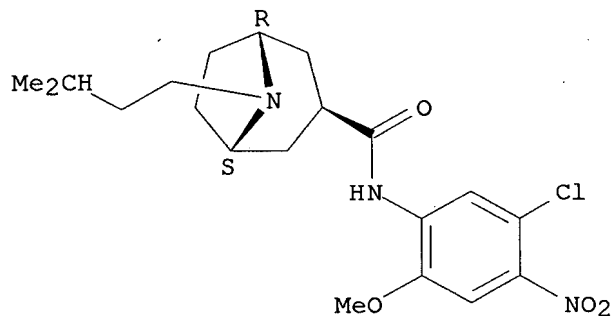
Relative stereochemistry.



RN 79522-17-1 CAPLUS

CN 8-Azabicyclo[3.2.1]octane-3-carboxamide, N-(5-chloro-2-methoxy-4-nitrophenyl)-8-(3-methylbutyl)-, exo- (9CI) (CA INDEX NAME)

Relative stereochemistry.

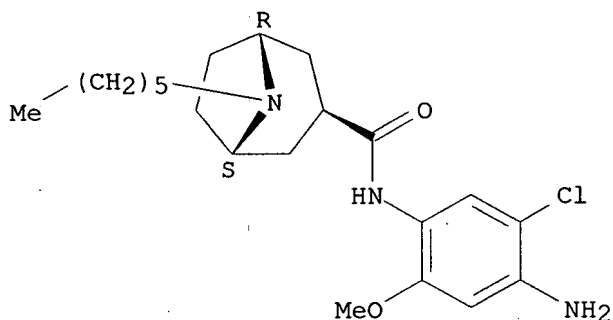


IT 79522-24-0P

RL: SPN (Synthetic preparation); PREP (Preparation)

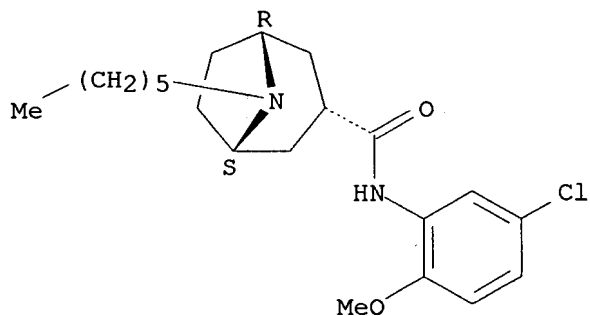
(preparation of)
 RN 79522-24-0 CAPLUS
 CN 8-Azabicyclo[3.2.1]octane-3-carboxamide, N-(4-amino-5-chloro-2-methoxyphenyl)-8-hexyl-, exo- (9CI) (CA INDEX NAME)

Relative stereochemistry.



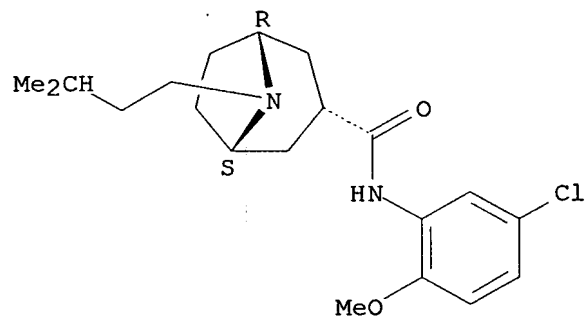
IT 79521-96-3 79521-97-4
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (N-alkylation by, of Me nortropanecarboxylate)
 RN 79521-96-3 CAPLUS
 CN 8-Azabicyclo[3.2.1]octane-3-carboxamide, N-(5-chloro-2-methoxyphenyl)-8-hexyl-, endo- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 79521-97-4 CAPLUS
 CN 8-Azabicyclo[3.2.1]octane-3-carboxamide, N-(5-chloro-2-methoxyphenyl)-8-(3-methylbutyl)-, endo- (9CI) (CA INDEX NAME)

Relative stereochemistry.



ACCESSION NUMBER: 1964:75528 CAPLUS
 DOCUMENT NUMBER: 60:75528
 ORIGINAL REFERENCE NO.: 60:13285h,13286a-h,13287a-c
 TITLE: 3-(Monocarbocyclic aryl)-3-carboxytropanes and esters thereof
 INVENTOR(S): Archer, Sydney; Bell, Malcolm R.
 PATENT ASSIGNEE(S): Sterling Drug Inc.
 SOURCE: 14 pp.
 DOCUMENT TYPE: Patent
 LANGUAGE: Unavailable
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3120537		19640204	US 1958-731857	19580430
PRIORITY APPLN. INFO.:			US	19580430

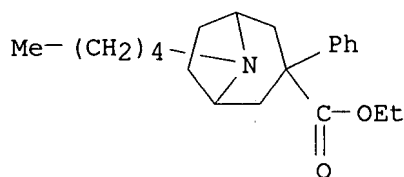
GI For diagram(s), see printed CA Issue.

AB The title compds. (I, R₁ = alkyl) are useful as analgesics. Thus, an aqueous solution of nortropinone hydrochloride and KCN, kept below 25°, formed the cyanohydrin which was hydrolyzed to the hydroxy acid (II, R = R₁ = H) in concentrated, aqueous HCl. The acid, after refluxing 20 hrs. in MeOH-HCl, formed

nor- α -ecgonine Me ester (II, R = H, R₁ = Me), m. 144-7° (EtOAc). The ester, refluxed with PhCH₂CH₂Br and KOAc, formed 8-(2-phenylethyl)nor- α -ecgonine Me ester (II, R = PhCH₂CH₂, R₁ = Me) which formed a hydrochloride, m. 223-9° (decomposition). Similarly, II Me esters (R₁ = Me) were prepared (R given): propargyl; p-H₂NC₆H₄CH₂CH₂; PhCH₂; PhCH₂CH₂CH₂; p-MeOC₆H₄CH₂CH₂; p-ClC₆H₄CH₂CH₂; cinnamyl (p-MeC₆H₄SO₃H salt m. 201-2°). A solution of α -ecgonine Me ester (II, R = R₁ = Me) in tetrahydrofuran (THF) was added to PhLi in Et₂O over 20 min. and the mixt refluxed 1 hr. to give the carbinol (III, R = Me, R₁ = R₂ = Ph), m. 116-17° (hexane); hydrochloride m. 279.5-80.5° (decomposition). Similarly, III were prepared [R, R₁, R₂, salt, m.p. (decomposition) of the salt given]: Me, m-MeOC₆H₄, m-MeOC₆H₄, HCl, 236-7°; H, Ph, Ph, HCl, 259.5°; PhCH₂CH₂, Ph, Ph, HCl, 271.5-4.0°; propargyl, Ph, Ph, --, --; p-H₂NC₆H₄CH₂CH₂, Ph, Ph, --, --; PhCH₂, Ph, Ph, --, --; PhCH₂CH₂CH₂, Ph, Ph, --, --; p-MeOC₆H₄CH₂CH₂, Ph, Ph, --, --; p-ClC₆H₄CH₂CH₂, Ph, Ph, --, --. II (R = R₁ = Me), and NaNH₂ in liquid NH₃ yielded 3-carbamoylpseudotropine, m. 155.8-9.2°, which, with EtMgBr in THF, formed 3-propionylpseudotropine (IV), m. 120.6-3.4°. IV and PhLi in THF formed III (CR = Me, R₁ = Ph, R₂ = Et), isolated as HCl salt, m. 212.4-13.8°. Thus, III was prepared (R, R₁, R₂, salt, m.p. of the salt given): Me, Et, m-MeOC₆H₄, HCl, 245.05.5° (decomposition). III (R = Me, R₁ = R₂ = Ph) with ZnCl₂ in Ac₂O at room temperature 80 min. formed V (β -series) (Va), m. 166.0-6.5° (Va.HCl m. 276-7°), while the same III, refluxed with Ac₂O 20 hrs., formed V (α -series) (Vb), m. 162.0-45.° (Vb.HCl m. 265-6°). Vb heated with ZnCl₂ in Ac₂O on a steam bath 1.5 hrs. formed VI (α -series, R = Me, R₁ = R₂ = Ph), m. 312° (decomposition), while Va with ZnCl₂ in Ac₂O at room temperature 54 hrs. formed VI (β -series, R = Me, R₁ = R₂ = Ph), m. 121.0-2.5° (HCl salt m. 249-51°; MeI salt m. 233.5-7.5°). The latter was also formed from III (R = Me, R₁ = R₂ = Ph) and ZnCl₂ in Ac₂O at room temperature 63 hrs. Other III, with ZnCl₂ in Ac₂O at room temperature, formed the following VI (R, R₁, R₂, m.p., salt, m.p. of the salt given): Me, m-MeOC₆H₄, m-MeOC₆H₄ (VII), --, --, --; H, Ph, Ph (VIII), 209-12°, HCl, 290.0-1.5° (decomposition); PhCH₂CH₂, Ph, Ph, 112-14°, HCl, 266-7° (decomposition); propargyl, Ph, Ph, --, --, --; p-H₂NC₆H₄CH₂CH₂, Ph, Ph, --, --, --; PhCH₂, Ph, Ph, --, --, --; PhCH₂CH₂CH₂, Ph, Ph, --, --, --; p-MeO-C₆H₄CH₂CH₂, Ph, Ph, --, --, --; p-ClC₆H₄CH₂CH₂, Ph, Ph, --, --, --; Me, Et, Ph, --, HCl, 273.2-5.8°; Me, Et, m-MeO-C₆H₄, --, HCl, 237.5-8.5°. VII

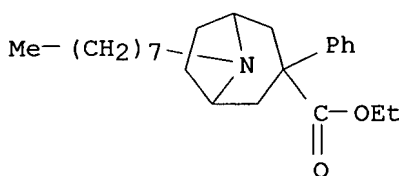
was demethylated with aqueous HBr to form the corresponding VI (R = Me, R1 = R2 = m-HO-C6H4). VI and H2NOH.HCl in pyridine and an alc. formed the oxime (IX). Thus, the following IX were prepared (R, R1, R2, m.p., salt, m.p. of the salt given): Me, Ph, Ph, --, HCl (β -series), 327° (decomposition); Me, Ph, Ph, --, -- (α -series), --; Me, p-MeOC6H4, p-MeOC6H4, --, HCl, 295° (decomposition); PhCH2CH2, Ph, Ph, --, HCl, 313-15°; propargyl, Ph, Ph, --, --, --; p-H2NC6H4CH2CH2, Ph, Ph, --, --, --; PhCH2, Ph, Ph, --, --, --; PhCH2CH2CH2, Ph, Ph, --, --, --; p-MeOC6H4CH2CH2, Ph, Ph, --, --, --; p-ClC6H4CH2CH2, Ph, Ph, --, --, --; Me, Et, Ph (XI), --, --, --; Me, Et, m-MeOC6H4 (XII), --, --, --. IX heated on a steam bath with HOAc and HCl .apprx.2 hrs. formed I (R1 = H) which was esterified by standing at room temperature in the appropriate R1OH 15 hrs. to several days. Thus, the following I were prepared (R, R1, R2, m.p., salt, m.p. of the salt given): Me, Et, Ph (XIII), 187-91°, MeBr (β -series), 206.0-7.5°; Me, H, Ph (XIV), --, HCl (β -series), 224-5°; Me, Me, Ph, --, -- (β -series), --; Me, iso-Pr, Ph, --, -- (β -series), --; Me, Pr, Ph, --, -- (β -series), --; Me, Bu, Ph, --, -- (β -series), --; Me, n-hexyl, Ph, --, -- (β -series), --; Me, H, Ph, --, -- (α -series), --; Me, Et, Ph, --, -- (α -series), --; Me, H, m-HOC6H4, --, --, --; Me, Et, m-HOC6H4, --, --, --; Me, H, m-MeOC6H4 (XV), 235° (decomposition), HCl, 215.0-17.5°; Me, Et, m-MeOC6H4, --, HBr, 178-80°; H, H, Ph (XVI), --, HCl, 275.0-6.5° (decomposition); H, Et, Ph (XVII), --, HCl, 219.521.5° (decomposition); PhCH2CH2, H, Ph, --, HCl, 224.0-4.5°; PhCH2-CH2, Et, Ph, --, HCl, 198.0-9.5°; propargyl, H, Ph, --, --, --; p-H2NC6H4CH2CH2, H, Ph, --, --, --; PhCH2, H, Ph, --, --, --; PhCH2CH2CH2, H, Ph, --, --, --; p-MeOC6H4CH2CH2, H, Ph, --, --, --; p-ClC6H4CH2CH2, H, Ph, --, --, --. Similarly, XI yielded XIV while XII yielded XV. XVI and SOCl2 formed the acid chloride which, with EtOH, formed XVII. XV was demethylated with aqueous HBr to the phenol (XVIII) which formed an HCl salt, m. 274.2-5.8°. XVIII in EtOH-HCl formed the Et ester (XIX) which, with acid chlorides or acid anhydrides, formed the corresponding Ph ester (XX). Thus, the XX were prepared (R given): Me, C5H11, HO2CCH2CH2, β -cyclopentylpropyl, Ph, PhCH2, 3,4,5 (MeO)3C6H2. XVII refluxed 17 hrs. with RBr and Na2CO3 in BuOH formed the corresponding I. Thus, I (R1 = Me, R2 = Ph) were prepared (R, salt, m.p. of the salt given): allyl, HCl, 193.5-4.0° (decomposition); cinnamyl, MeSO3H, 178.0-80.5°; PhNHCH2CH2, p-MeC6H4SO3H, 194-5°; n-C8H17, HCl, 138.8-46.0°; n-C5H11, HCl, 148.6-55.4°; propargyl, --, --; p-H2NC6H4CH2CH2, --, --; PhCH2, --, --; PhCH2CH2CH2, --, --; p-MeOC6H4CH2CH2, --, --; p-ClC6H4CH2CH2, --, --; cyclopropyl, --, --; cyclopropylmethyl, --, --; Et, --, --; PH2C(CN)CH2CH2, --, --. VI (R = Me, R1 = R2 = Ph, β -series), when reduced with LiAlH4 in refluxing Et2O 6 hrs., formed the corresponding carbinol (XXI), m. 160-1° (MeI salt m. 280.0-2.5°). VI in EtOH was also hydrogenated over PtO2 to XXI. VIII, when heated 5 hrs. with CNBr in benzene at 50-5° formed the corresponding N-cyano derivative, m. 160.5-2.5° which was reconverted to VIII by hydrolysis with aqueous HCl. Certain of the intermediates (I, R1 = H III V VI IX XXI) for the preparation of the title compds. are useful as anticholinergic or ganglionic blocking agents.

IT 95007-06-0P, 3-Nortropanecarboxylic acid, 8-pentyl-3-phenyl-, ethyl ester, hydrochloride 95749-73-8P, 3-Nortropanecarboxylic acid, 8-octyl-3-phenyl-, ethyl ester, hydrochloride
 RL: PREP (Preparation)
 (preparation of)
 RN 95007-06-0 CAPLUS
 CN 3-Nortropanecarboxylic acid, 8-pentyl-3-phenyl-, ethyl ester, hydrochloride (7CI) (CA INDEX NAME)



● HCl

RN 95749-73-8 CAPLUS
 CN 3-Nortropanecarboxylic acid, 8-octyl-3-phenyl-, ethyl ester, hydrochloride
 (7CI) (CA INDEX NAME)



● HCl

L4 ANSWER 25 OF 28 CAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 1963:73513 CAPLUS
 DOCUMENT NUMBER: 58:73513
 ORIGINAL REFERENCE NO.: 58:12613f-h,12614a-e
 TITLE: 3-Hydroxy-3-[(monocarbocyclic aryl)hydroxymethyl]tropanes
 INVENTOR(S): Archer, Sydney; Bell, Malcolm
 PATENT ASSIGNEE(S): Sterling Drug Inc.
 SOURCE: 14 pp.
 DOCUMENT TYPE: Patent
 LANGUAGE: Unavailable
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 3073829		19630115	US	19600108
PRIORITY APPLN. INFO.:			US	19600108

GI For diagram(s), see printed CA Issue.

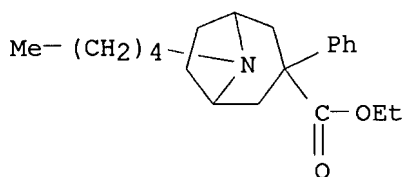
AB Cf. the following abstract The compds. prepared have analgetic activity. A solution of 100 g. α -ecgonine Me ester in 325 ml. tetrahydrofuran was added during 20 min. to a stirred solution of PhLi (prepare from 316 g. PhBr and 27.9 g. Li wire) in 1 l. Et₂O (vigorous reflux), the mixture stirred and refluxed 1 hr., then cooled and treated with 300 ml. H₂O, the solid filtered off, washed with Et₂O, the dark red filtrates decolorized with active C, dried (Na₂SO₄), treated with excess alc. HCl, and the precipitate filtered off and dried at 60° in vacuo 15 hrs. to give 167 g. I, HCl salt m. 279.5-80.5° (decomposition) (MeOH-Et₂O). A sample of I was treated with aqueous Na₂CO₃ to give the free base, m. 116-17° (hexane). Fused, powdered ZnCl₂ (10 g.) was added all at once to a stirred suspension of 10 g. I in 25 ml. (MeCO)₂O at room temperature, the mixture which became homogeneous after 50 min., stirred 80 min. poured into a solution of 25 g.

NaOH in 200 ml. H₂O, the tan solid collected, dried, extracted with 250 ml. boiling Me(CH₂)₄Me, concentrated to 100 ml., this cooled, and filtered to give 4.7 g. crystalline powder, m. 155-60°; the filtrate was concentrated to give an addnl. 1 g. The 2 crops were combined and recrystd. from 30 ml. boiling MeOH to give 4.3 g. 3-benzhydrylidene-tropene epoxide (II), plates, m. 166-6.5°; HCl salt m. 276-7° (decomposition) (MeOH-Et₂O). The ultraviolet spectrum of II showed ϵ 13,400, λ 220 m μ , and weak absorption peaks at 250-60 m μ . Similarly prepared were the following compds. (m.p. given): 3-phenyl-3-benzoyltropene, 121-2.5° (hexane), HCl salt 249-51° (absolute alc.), methiodide m. 233.5-7.5°; 3-phenyl-3-(phenylisonitrosomethyl)tropene-HCl, 327° (decomposition); 3-phenyl-3-carboxytropene-HCl, 224-5° (decomposition) (MeOH-Et₂O); 3-phenyl-3-carbethoxytropene-HCl, 187-91° (decomposition), methobromide, 206-7° (iso-PrOH-Et₂O); 3-[di(m-anisyl)hydroxymethyl]pseudotropine, 236-7° (decomposition) (iso-PrOH-Et₂O); 3-(m-anisyl)-3-(m-anisoyl)tropene showed a strong peak at 6.02 m μ ; 3-(m-anisyl)-3-[(m-anisyl)isonitrosomethyl]-tropene-HCl, 295° (decomposition) (H₂O); 3-(m-anisyl)-3-carboxytropene-HCl, 215-17.5° (PrOH-Et₂O); 3-(m-anisyl)-3-carbethoxytropene-HBr, 178-80° (alc.-Et₂O); nor- α -ecgonine Me ester, 144-7° (AcOEt); 3-(diphenylhydroxymethyl)(norpseudotropine-HCl), 259.5° (decomposition) (PrOH), it contains PrOH of crystallization; 3-phenyl-3-benzoylnortropene, 209-12° (PrOH); HCl salt 290-1.5° (decomposition) (PrOH-Et₂O); 8-cyano-3-phenyl-3-benzoylnortropene, 160.5-2.5° (MeOH); 3-phenyl-3-(phenylisonitrosomethyl)nortropene-HCl, 286° (decomposition) (H₂O); 3-phenyl-3-carbethoxynortropene-HCl, 219.5-21.5° (decomposition) (alc.-Et₂O); 8-allyl-3-phenyl-3-carbethoxynortropene-HCl, 193.5-94° (decomposition) (iso-PrOH-Et₂O); 8-cinnamyl-3-carbethoxy-3-phenylnortropene methanesulfonate, 178-80.5° (iso-PrOH-Et₂O); 8-(2-phenylaminoethyl)-3-phenyl-3-carbethoxynortropene p-toluenesulfonate, 194-5° (PrOH); 8-(n-octyl)-3-phenyl-3-carbethoxynortropene-HCl, 38.8-46° (CCl₄-Et₂O); 8-(2-phenylethyl)nor- α -ecgonine Me ester-HCl, 223-9° (decomposition) (alc.-Et₂O); 8-(2-phenylethyl)-3-(diphenylhydroxymethyl)(norpseudotropine-HCl, 271.5-74° (decomposition) (MeOH-Et₂O); 8-(2-phenylethyl)-3-phenyl-3-benzoylnortropene, 112-14° (hexane); HCl salt, 266-7° (decomposition) (absolute alc.); 8-(2-phenylethyl)-3-phenyl-3-(phenylisonitrosomethyl)nortropene-HCl, 313-15° (HCONMe₂); 8-(2-phenylethyl)-3-phenyl-3-carboxynortropene-HCl, 224-4.5° (Me-OH-Et₂O); 8-(2-phenylethyl)-3-phenyl-3-carbethoxynortropene-HCl, 198-9.5° (MeOH-Et₂O); 8-cinnamylnor- α -ecgonine Me ester p-toluenesulfonate, 201-2° (iso-PrOH); 3-phenyl-3-(phenylhydroxymethyl)tropene, 160-1° (CCl₄); methiodide, 280-2.5°; 3-carbamylpseudotropine, 155.8-9.2°; 3-propionylpseudotropine, 120.6-3.4° (hexane); 3-(ethylphenylhydroxymethyl)pseudotropine-HCl, 212.4-13.8° (MeOH-Et₂O); 3-phenyl-3-propionyltropene-HCl, 273.2-5.8° (MeOH-Et₂O); 3-[ethyl(m-anisyl)hydroxymethyl]pseudotropine - HCl, 245-5.5° (decomposition) (MeOH-Et₂O); 3-(m-anisyl)-3-propionyltropene-HCl, 237.5-8.5° (iso-PrOH-Et₂O); 3-(m-hydroxyphenyl)-3-propionyltropene-HCl, 274.2-5.8° (alc.-Et₂O).

IT 95007-06-0P, 3-Nortropanecarboxylic acid, 8-pentyl-3-phenyl-, ethyl ester, hydrochloride 95749-73-8P, 3-Nortropanecarboxylic acid, 8-octyl-3-phenyl-, ethyl ester, hydrochloride
 RL: PREP (Preparation)
 (preparation of)

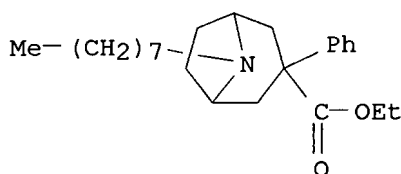
RN 95007-06-0 CAPLUS

CN 3-Nortropanecarboxylic acid, 8-pentyl-3-phenyl-, ethyl ester, hydrochloride (7CI) (CA INDEX NAME)



● HCl

RN 95749-73-8 CAPLUS
 CN 3-Nortropanecarboxylic acid, 8-octyl-3-phenyl-, ethyl ester, hydrochloride
 (7CI) (CA INDEX NAME)



● HCl

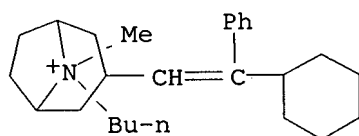
L4 ANSWER 26 OF 28 CAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 1958:93024 CAPLUS
 DOCUMENT NUMBER: 52:93024
 ORIGINAL REFERENCE NO.: 52:16402b-f
 TITLE: 8-Alkyl nortropane derivatives
 INVENTOR(S): Zirkle, Charles L.
 PATENT ASSIGNEE(S): Smith, Kline & French Laboratories
 DOCUMENT TYPE: Patent
 LANGUAGE: Unavailable
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2800482		19570723	US 1955-519650	19550701

AB 3-Benzhydrylidene tropane picrate m. 237-8° (aqueous alc.); methobromide, m. 281-5° (iso-PrOH-Me₂CO); etho(ethyl sulfate), white solid. Di(2-thienyl)-3-tropanylcarbinol (0.5 g.) in CHCl₃ treated with dry HCl until strongly acid gave 2-[di(2-thienyl)methylidene]tropane-HCl, m. 224-5° (alc. Et₂O). 1,1-Di(2-thienyl)-3-tropaneethanol (1 g.), 2 g. (CO₂H)₂, and 3 ml. H₂O refluxed 2 hrs. gave 1,1-di(2-thienyl)-2-(3-tropanyl)ethylene, m. 74-6° (ligroine); picrate, m. 190-2° (aqueous Me₂CO); HCl salt, m. 230-2° (alc. Et₂O); methobromide, m. 252-3°. 1,1-Diphenyl-2-(3-tropanyl)ethylene methobromide, m. 286° (alc.); maleate; metho-p-toluene-sulfonate, white solid. 1-Phenyl-1-(2-thienyl)-3-tropaneethanol (9.7 g.), 19.4 g. (CO₂H)₂, and 29 ml. H₂O refluxed 2 hrs. and the mixture made alkaline gave 1-phenyl-1-(2-thienyl)-2-(3-tropanyl)ethylene, m. 69-72°; picrate, m. 209-10°; tartrate, m. 174-5° (alc.-Et₂O); methobromide, m. 258-9° (alc.-Et₂O). 1-Phenyl-1-(2-pyridyl)-2-(3-tropanyl)ethylene methobromide, m. 228-30° (alc.-Et₂O); tartrate, m. 165-7° (alc.-Et₂O). 1-(2-Cyclohexylethyl)-1-phenyl-3-

tropaneethanol (1 g.) in 10 ml. AcOH and 3 ml. 37% HCl refluxed 0.5 hr. gave the dehydration product, λ 235 m μ , log ϵ 3.58. 1-Cyclohexyl-1-phenyl-2-(3-tropanyl) ethylene-HI, m. 222.5-4.0°; methobromide, m. 250-3° (H2O); butiodide, white solid. 1,1-Diphenyl-3-tropanepropanol (15 g.) in 50 ml. 37% HCl 1.5 hrs. at 100° gave 1,1-diphenyl-3-(3-tropane-1-propene, m. 59-60°, b0.4 170-3°; citrate, m. 174°. 1-(2-Pyridyl-1-p-tolyl-4-(3-tropanyl)-1-butanol (0.5 g.) and 2 ml. 85% H2SO4 heated 15 min. at 155° gave 1-(2-pyridyl)-1-p-tolyl-4-(3-tropanyl)-1-butene. A similar dehydration of 1-cyclopentyl-1-phenyl-3-tropanebutanol with HCl gave the corresponding butene as the HCl salt; neutralization with NH4OH gave the free base as a yellow oil.

IT 124111-32-6P, 8-Butyl-3-(β -cyclohexylstyryl)tropanium iodide
 RL: PREP (Preparation)
 (preparation of)
 RN 124111-32-6 CAPLUS
 CN 8-Butyl-3-(β -cyclohexylstyryl)tropanium iodide (6CI) (CA INDEX NAME)



● I⁻

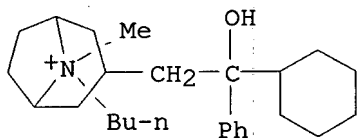
L4 ANSWER 27 OF 28 CAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 1958:93023 CAPLUS
 DOCUMENT NUMBER: 52:93023
 ORIGINAL REFERENCE NO.: 52:16401g-i,16402a-b
 TITLE: 8-Alkyl-nortropane derivatives
 INVENTOR(S): Zirkle, Charles L.
 PATENT ASSIGNEE(S): Smith, Kline & French Laboratories
 DOCUMENT TYPE: Patent
 LANGUAGE: Unavailable
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2800481		19570723	US 1955-519649	19550701

AB Me 3-tropanecarboxylate (10.1 g.) in 100 ml. Et2O stirred 1.5 hrs. at room temperature with PhLi gave diphenyl-3-tropanylcarbinol, m. 214-15° (aqueous MeOH); citrate, m. 112-18° (iso-PrOH-Et2O); methobromide, m. 309-10° (alc.). Et 3-tropaneacetate (I) (10 g.) in 20 ml. Et2O refluxed with PhLi and 11.8 g. thiophene in Et2O gave 1,1-di(2-thienyl-3-tropaneethanol, m. 138-40° (EtOAc); acetate, m. 189-90°; methobromide, m. 245.5° (alc.). 1,1-Diphenyl-3-tropaneethanol-HCl, m. 234-5° (alc.-Et2O); methobromide, m. 282-3° (alc.-Et2O). I with concentrated HCl gave 3-tropaneacetic acid-HCl (II), m. 172-4°. II (11 g.) refluxed with PhLi gave Ph 3-tropanylmethyl ketone (III), b0.2 138-41°. III (9 g.) stirred several hrs. at room temperature with PhLi gave 1,1-diphenyl-3-tropaneethanol-HBr, m. 230°. III (10 g.) treated with PhLi and thiophene gave 1-phenyl-1-(2-thienyl)-3-tropaneethanol, m. 137.5-9.0°; maleate, m. 145-6° (alc.-Et2O); methobromide, m. 256° (alc.). 1-Phenyl-1-(2-pyridyl)-3-tropaneethanol-HI, m. 194-6°; methobromide, m. 268°

(alc.). 1-Ethyl-1-phenyl-3-tropaneethanol-HCl, m. 237-7.5° (alc.). 1-Cyclohexyl-1-phenyl-3-tropaneethanol-HCl, m. 254-5° (alc.-Et2O); methobromide, m. 262° (alc.-Et2O). 2-Cyclohexylethyl 3-tropanylmethyl ketone picrate, m. 148-50°; 1-(2-cyclohexylethyl)-1-phenyl-3-tropaneethanol-HCl, m. 215-16°; citrate, m. 134-6° (Me2CO-MeOH); methobromide, m. 263-5°. II (3.7 g.) treated with SOCl2 gave the acid chloride HCl salt which treated with CH2N2 gave the diazomethyl 3-tropanylmethyl ketone and subsequent treatment with Ag2O oxide gave Et 3-tropanepropionate (IV). IV (18 g.) treated with PhLi as above gave 1,1-diphenyl-3-tropanepropanol, m. 141-2.5°; HCl salt, m. 249-50°; methobromide salt, m. 299°. Cyclopentyl 3-(3-tropanyl)propyl ketone (6.6 g.) treated with PhLi as above gave 1-cyclopentyl-1-phenyl-3-tropanebutanol. Diphenyl-3-tropanecarbinol etho(ethyl sulfate) was a white solid. 1,1-Diphenyl-3-tropaneethanol metho-p-toluenesulfonate, m. 172-4°; etho(ethyl sulfate), m. 234-5°; butobromide, m. 225-7°; butiodide, m. 227-9°. 1-Cyclohexyl-1-phenyl-2-(3-tropane)ethanol butyl bromide was a white solid.

IT 119640-59-4P, 8-Butyl-3-(β-cyclohexyl-β-hydroxyphenethyl)tropanium bromide
 RL: PREP (Preparation)
 (preparation of)
 RN 119640-59-4 CAPLUS
 CN 8-Butyl-3-(β-cyclohexyl-β-hydroxyphenethyl)tropanium bromide
 (6CI) (CA INDEX NAME)



● Br⁻

L4 ANSWER 28 OF 28 CAPLUS COPYRIGHT 2007 ACS on STN
 ACCESSION NUMBER: 1958:93020 CAPLUS
 DOCUMENT NUMBER: 52:93020
 ORIGINAL REFERENCE NO.: 52:16399b-i,16400a-i,16401a
 TITLE: 8-Alkyl nortropane derivatives
 INVENTOR(S): Zirkle, Charles L.
 PATENT ASSIGNEE(S): Smith, Kline & French Laboratories
 DOCUMENT TYPE: Patent
 LANGUAGE: Unavailable
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2800478		19570723	US 1955-519646	19550701

AB Some new physiologically active 3-substituted-8-alkyl nortropanes, the nontoxic organic and inorg. salts, and the quaternary ammonium salts are described. Me 3-(3-hydroxytropane)carboxylate (10 g.) in 50 ml. Ac2O heated 4 hrs. at 100°, the excess Ac2O and AcOH removed in vacuo, the residue poured into H2O, extracted with Et2O, and the Et2O evaporated gave

Me 3-(3-acetoxytropane)-carboxylate (I), m. 66-7°, b15 162-5°.
 I (29 g.) added dropwise during 7 min. to a vertical tube heated to

420° and filled with pieces of Pyrex tubing, the apparatus swept with N, the product dissolved in dilute HCl, extracted with Et2O, the aqueous acid solution

saturated with K2CO3, and the product separated gave Me

3-(2-tropene)carboxylate

(II), b15 131-4°, n25.5D 1.4998. II (13 g.) in 100 ml. MeOH hydrogenated over 5 g. Raney Ni at 50 lb./sq. in. at room temperature and the mixture distilled gave Me 3-tropanecarboxylate (III), b18 128-32°, n25D 1.4819. III (10.1 g.) in 100 ml. Et2O stirred 1.5 hrs. at room temperature

with

a solution of PhLi (from 34.5 g. PhBr and 3.5 g. Li) in 100 ml. Et2O, the mixture added to 150 ml. H2O, and the solid collected and purified gave diphenyl-3-tropanecarbinol (IV), m. 185.5-6.0° (EtOAc). IV (5.6 g.) in 20 ml. AcOH and 25 ml. dilute HCl refluxed 10 min. and evaporated to dryness gave 3-benzhydrylidene-tropane-HCl, m. 275-8° (alc.-Et2O); free base (V), a colorless oil. V (4 g.) in alc. hydrogenated over Raney Ni at 400 lb./sq. in. at 60° and the product chromatographed on Al2O3 gave 3-benzhydryltropane (VI), m. 70-2°. VI (1 g.) gave the HCl salt, unmelted below 310°; MeBr salt, m. 277-9°; etho(ethyl sulfate), white solid. Tropinone (13.9 g.), 11.3 g. NCCH2CO2Et, 1.6 g. NH4OAc, 7.3 g. AcOH, 20 ml. alc., and 0.6 g. Pd-C shaken under H at 50° and 60 lb./sq. in. gave Et α-cyano-3-tropaneacetate (VII), b0.3 116-18°, n24D 1.4942. VII (8 g.) in 30 ml. 37% HCl refluxed 13 hrs. and the crude 3-tropaneacetic acid-HCl esterified by leaving 3 days at room temperature in 50 ml. alc. with dry HCl gave Et 3-tropaneacetate (VIII), b2 104-5°, n25D 1.4774. VIII (42 g.) in 100 ml. Et2O similarly treated with PhLi gave 1,1-diphenyl-3-tropaneethanol (IX), m. 146.5-7.5° (EtOAc). IX (14.6 g.) in 29 ml. 37% HCl and 100 ml. AcOH refluxed 0.5 hr. gave 1,1-diphenyl-2-(3-tropanyl)ethylene (X), as the HCl salt, m. 217-18° (alc.-Et2O); free X, m. 109.5-10.0° (Me2CO). X (10 g.) in alc. hydrogenated over Raney Ni at 500 lb./sq. in. and 60° gave 1,1-diphenyl-2-(3-tropanyl)ethane, colorless oil; HCl salt, m. 244-5°; methobromide, m. 257-8° (alc.-Et2O); metho-p-toluenesulfonate, white solid; maleate, obtained by treating with maleic acid in alc. VIII in 37% HCl refluxed several hrs. gave 3-tropaneacetic acid-HCl (XI), m. 172-4° (MeOH-Et2O). XI (11 g.) similarly treated with PhLi followed by passage of HCl gave the HCl salt which when washed was reconverted to phenyl 3-tropanylmethyl ketone (XII), b0.2 138-41°. BuLi (from 3.7 g. BuCl and 0.7 g. Li) in 25 ml. Et2O treated slowly at -45° with 5.5 g. 2-bromopyridine in 10 ml. Et2O, the mixture stirred 10 min., and 2.5 g. XII in 30 ml. Et2O added slowly, the mixture stirred 15 min. at -15°, 50 ml. H2O added, the mixture stirred a further 15 min., a solid collected, the solid stirred with CHCl3 and H2O, and the CHCl3 layer removed, combined with the Et2O layer and evaporated gave 1-phenyl-1-(2-pyridyl)-3-tropaneethanol (XIII), m. 117-18.5° (EtOAc). XIII (1 g.) and 2 ml. 85% H2SO4 heated 15 min. at 155° and the solution made basic gave 1-phenyl-1-(2-pyridyl)-2-(3-tropanyl)ethylene (XIV), m. 97.5-9.5° (Me2CO). XIV 0.2 g.), 5 g. cyclohexene, and 0.3 g. 20% Pd-C refluxed 48 hrs. gave 1-phenyl-1-(2-pyridyl)-2-(3-tropanyl)ethane (XV) as a thick oil; picrate, m. 201-3° (aqueous Me2CO). XV also forms the tartrate, m. 78-80° (alc.-Et2O). XII (12.2 g.) in 50 ml. Et2O added slowly to EtMgBr solution (from 7.3 g. Mg) at 0°, the mixture stirred 1.5 hrs. at room temperature, then refluxed 1.5 hrs., decomposed with ice and 21 g. NH4Cl

in

50 ml. H2O, the Et2O layer removed, and the aqueous phase extracted with CHCl3 gave 1-ethyl-1-phenyl-3-tropaneethanol (XVI), m. 119-20°. XVI (0.44 g.) was dehydrated by heating 40 min. at 100° with 3 ml. concentrated HCl to the ethylene, m. 170-200°. The ethylene hydrogenated in alc. over Raney Ni at 60° and 500 lb./sq. in. gave 1-ethyl-1-phenyl-2-(3-tropanyl)ethane (XVII), an oil, which formed an HCl salt. VIII (15 g.) similarly treated with 2-cyclohexylethylmagnesium

bromide gave 2-cyclohexylethyl 3-tropanylmethyl ketone (XVIII), b0.7 157-64°, n_D24.5D 1.5010. XVIII (7.7 g.) in 20 ml. Et₂O similarly treated with PhLi (from 9.5 g. PhBr) in Et₂O at 0° gave 1-(2-cyclohexylethyl)-1-phenyl-3-tropaneethanol (XIX), m. 104-6° (EtOAc). XIX (0.5 g.), 1 ml. HI, 3 ml. AcOH, and 0.13 g. red P refluxed 3.5 hrs., the solution filtered, the filtrate diluted with H₂O, the crude HI salt separated as an oil and crystallized gave

1-(2-cyclohexylethyl)-1-phenyl-2-(3-tropanyl)ethane-HI, m. 175° (alc.-Et₂O). The free base was a colorless oil; HCl salt, m. 198-200°. Similarly, 25 g. VIII reacted with cyclohexylmagnesium bromide to give cyclohexyl 3-tropanylmethyl ketone (XX), b0.9-1.1 142-53°, crystallizing to a white solid on standing. XX (10 g.) similarly treated with PhLi gave 1-cyclohexyl-1-phenyl-3-tropaneethanol (XXI), m. 139-40.5° (EtOAc). XXI (1 g.) refluxed 0.5 hr. with AcOH and concentrated HCl gave the ethylene

HCl

salt, m. 195-6°. Hydrolysis gave the free base as an oil. The free base (4.4 g.) hydrogenated over Raney Ni at 500 lb./sq. in. and 60° gave 1-cyclohexyl-1-phenyl-2-(3-tropanyl)ethane, colorless oil; HCl salt, m. 167-8.5°; citrate, m. 153-5°; butiodide, white solid. N-Isopropyl-nortropanone (16.7 g.), 11.3 g. NCCH₂CO₂Et, 1.6 g. NH₄OAc, 7.3 g. AcOH, 20 ml. alc., and 0.6 g. Pd-C shaken with H at 60 lb./sq. in. and 60°, the residue refluxed 12 hrs. with concentrated HCl gave crude 3-(N-isopropyl-nortropane)-acetic acid-HCl which was esterified with anhydrous MeOH and HCl 3 days at room temperature gave Me 3-(N-isopropyl-nortropane)acetate (XXII), b0.3 124-7°. XXII (11.3 g.) similarly treated with p-anisylmagnesium bromide gave p-anisyl 3-(N-isopropyl-nortropanyl)methyl ketone (XXIII), b0.2 160-4° and crystallized as a white solid. XXIII (7.5 g.) similarly treated with PhLi at 0° gave 1-(p-anisyl)-1-phenyl-3-(N-isopropyl-nortropane)ethanol (XXIV), white solid. Dehydration of XXIV with oxalic acid and H₂O gave the ethylene, which when hydrogenated as described above gave 1-p-anisyl-1-phenyl-2-[3-(N-isopropyl-nortropanyl)]ethane; methobromide salt. VIII (164 g.) in 500 ml. Et₂O refluxed 3 hrs. with 30 g. LiAlH₄ in 2 l. Et₂O gave 3-tropaneethanol (XXV), m. 63-4° (C₆H₆-ligroine). XXV (10 g.) in 50 ml. CHCl₃ treated with 14.3 g. SOCl₂, refluxed 45 min., and isolation gave 1-chloro-2-(3-tropanyl)ethane-HCl, m. 167-8° (alc.-Et₂O); free base, b0.9 81°. The base (47 g.) and 0.1 g. NaI refluxed 17 hrs. with 49 g. KCN in 175 ml. alc. and 75 ml. H₂O, NaOH added to the residual mixture, and the product isolated gave 3-tropanepropionitrile (XXVI), b0.3 114-16°, n_D25D 1.4958. XXVI (25 g.) in 100 ml. 37% HCl refluxed several hrs., and evaporated, the residue dissolved in 300 ml. alc., 5 ml. concentrated H₂SO₄ added, and the residue treated with 40% NaOH gave Et 3-tropanepropionate (XXVII), b0.4 97-100°, n_D25D 1.4770. Similarly XXVII treated with PhLi gave 1,1-diphenyl-3-tropanepropanol (XXVIII), m. 141-2.5°. Dehydration of XXVIII with concentrated HCl and 40% NaOH added gave 1,1-diphenyl-3-(3-tropanyl)-1-propene (XXIX), b0.4 170-3°, m. 59-60°. XXIX (4.7 g.) hydrogenated over 5 g. Raney Ni gave 1,1-diphenyl-3-(3-tropanyl)propane as an oil; citrate, m. 170°; methobromide, m. 277°. XXVII reduced with 3 g. LiAlH₄ gave 3-tropanepropanol (XXX), b2 128-31°. XXX (7.7 g.) treated with 10 g. SOCl₂ gave the HCl salt, which treated with K₂CO₃ liberated 1-chloro-3-(3-tropanyl)propane (XXXI), b1 100-2°. XXXI (5 g.) refluxed 18 hrs. with 0.1 g. NaI, 5 g. KCN, 18 ml. alc., and 8 ml. H₂O gave 3-tropanebutyronitrile (XXXII), b0.3 132-5°. XXXII (3 g.) refluxed several hrs. with concentrated HCl and the product treated with 40% NaOH gave Et 3-tropanebutyrate (XXXIII), b0.5 115-19°. XXXIII (2.3 g.) similarly treated with p-tolyl magnesium bromide gave p-tolyl γ-(3-tropanyl)propyl ketone (XXXIV), b0.2 188-92°. XXXIV (1.5 g.) in 15 ml. Et₂O treated with BuLi and 2-bromopyridine in Et₂O gave 1-(2-pyridyl)-1-p-tolyl-3-tropanebutanol (XXXV), crystalline solid. XXXV (0.5 g.) dehydrated with 85% H₂SO₄, and the product reduced as described above gave 1-(2-pyridyl)-1-p-tolyl-4-(3-

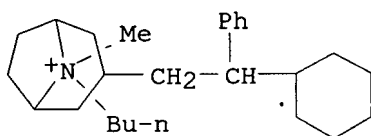
tropanyl)butane. II (9.2 g.) with MeLi gave dimethyl-3-tropanecarbinol, which was dehydrated by refluxing with AcOH and concentrated HCl, and the product hydrogenated over Raney Ni to give 3-isopropyltropane as an oil. XXII (11.3 g.) treated with C₆H₁₃Li gave 1,1-dihexyl-3-(N-isopropyl-nortropane)ethanol (XXXVI), white solid. XXXVI (8 g.) refluxed 45 min. with AcOH and HCl gave an unsatd. product as the HCl salt which was hydrogenated over Raney Ni to 2-hexyl-1-[3-(N-isopropyl-nortropanyl)]octane as an oil. XXXIII (14.3 g.) similarly treated with cyclopentylmagnesium bromide gave cyclopentyl 3-(3-tropanyl)propyl ketone (XXXVII), b_{0.9} 152-6°. XXXVII (3.5 g.) dehydrated and the product reduced over Raney Ni gave 1-cyclopentyl-1-phenyl-4-(3-tropanyl)butane, a colorless oil.

IT 119640-62-9P, 8-Butyl-3-(β-cyclohexylphenethyl)tropanium iodide

RL: PREP (Preparation)
(preparation of)

RN 119640-62-9 CAPLUS

CN 8-Butyl-3-(β-cyclohexylphenethyl)tropanium iodide (6CI) (CA INDEX NAME)



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=> FIL STNGUIDE

COST IN U.S. DOLLARS

SINCE FILE ENTRY	TOTAL SESSION
150.16	322.47

FULL ESTIMATED COST

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE ENTRY	TOTAL SESSION
-21.84	-21.84

CA SUBSCRIBER PRICE

FILE 'STNGUIDE' ENTERED AT 08:48:55 ON 06 JUN 2007

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LAST RELOADED: Jun 4, 2007 (20070604/UP).

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FILE 'REGISTRY' ENTERED AT 08:42:34 ON 06 JUN 2007

L1 STRUCTURE UPLOADED

L2 4 S L1

L3 133 S L1 FULL

FILE 'CAPLUS' ENTERED AT 08:43:13 ON 06 JUN 2007

L4 28 S L3 FULL

FILE 'STNGUIDE' ENTERED AT 08:48:55 ON 06 JUN 2007

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COST IN U.S. DOLLARS

SINCE FILE
ENTRY

TOTAL
SESSION

FULL ESTIMATED COST

0.72

323.19

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE
ENTRY

TOTAL
SESSION

CA SUBSCRIBER PRICE

0.00

-21.84

STN INTERNATIONAL LOGOFF AT 08:56:24 ON 06 JUN 2007